

FIG. 1(a)

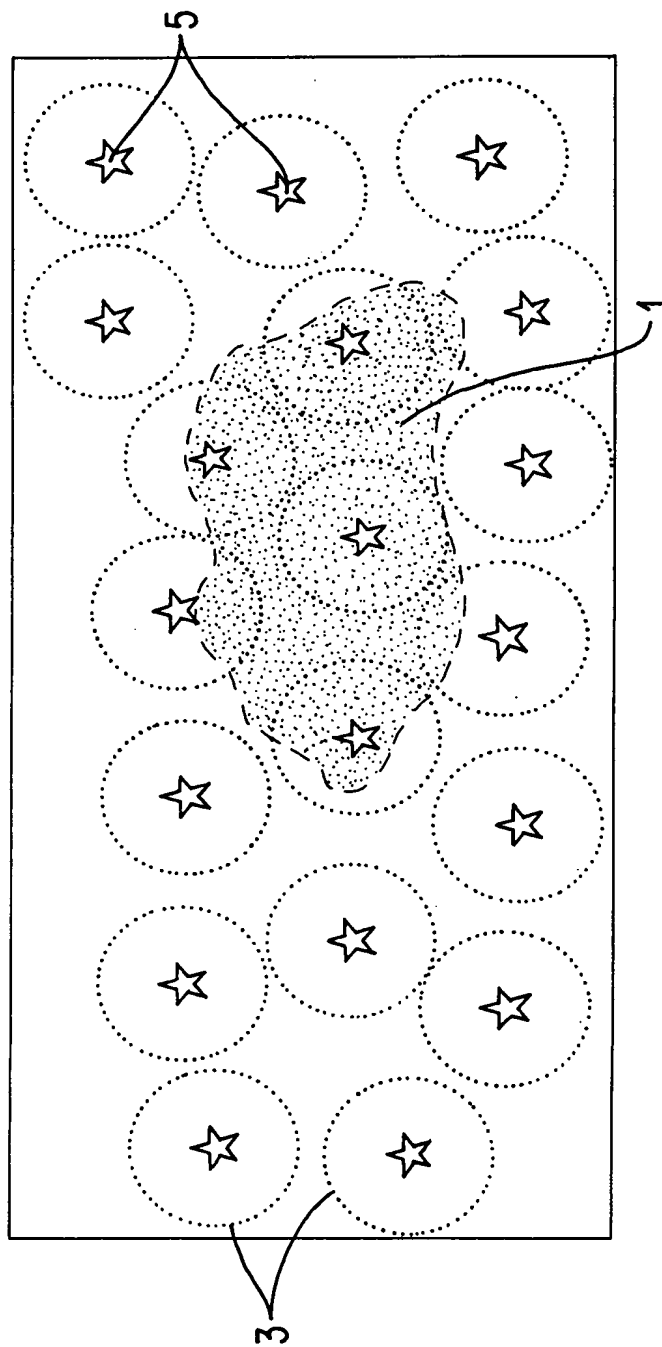


FIG. 1(b)

105250" E4999860

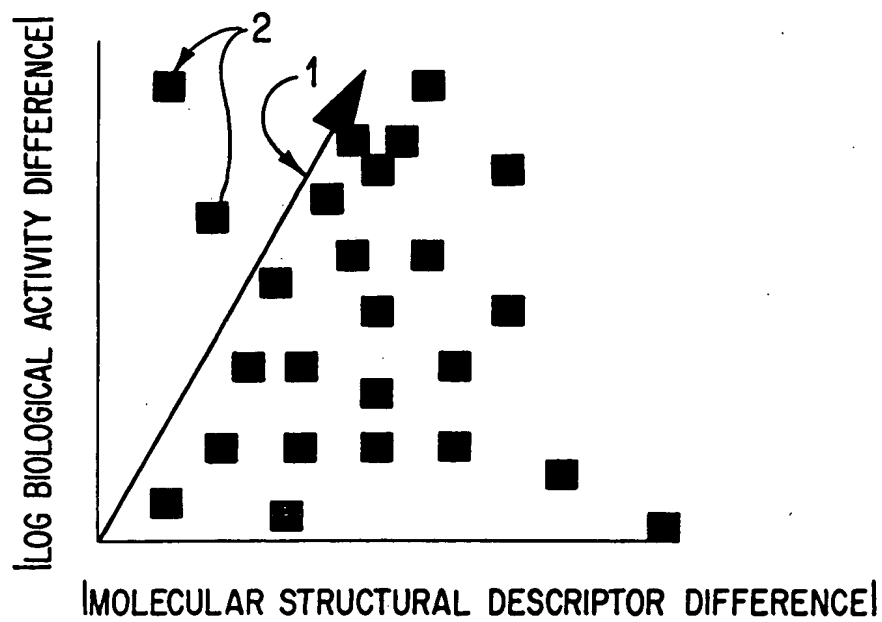


FIG. 2

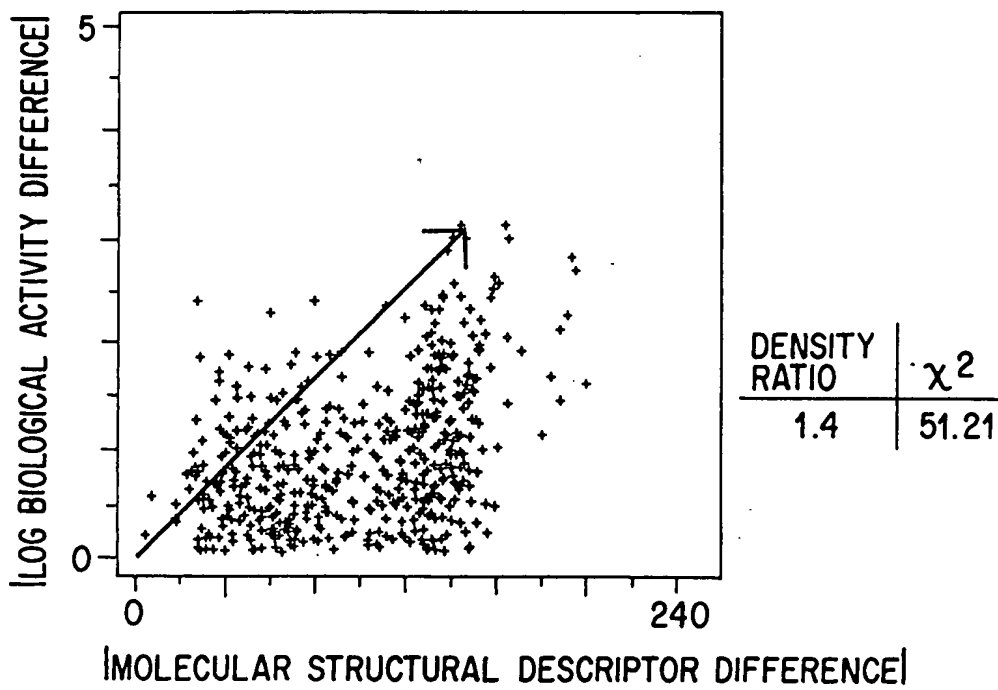
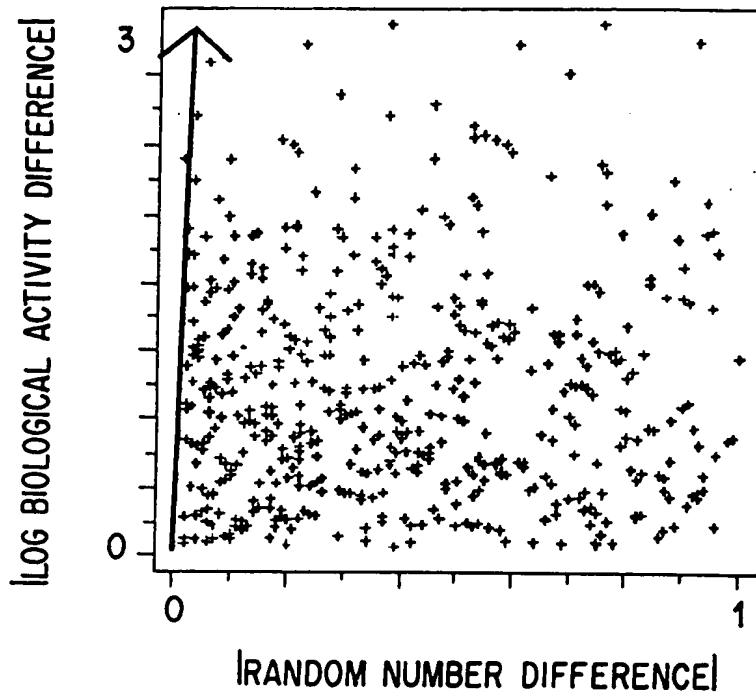
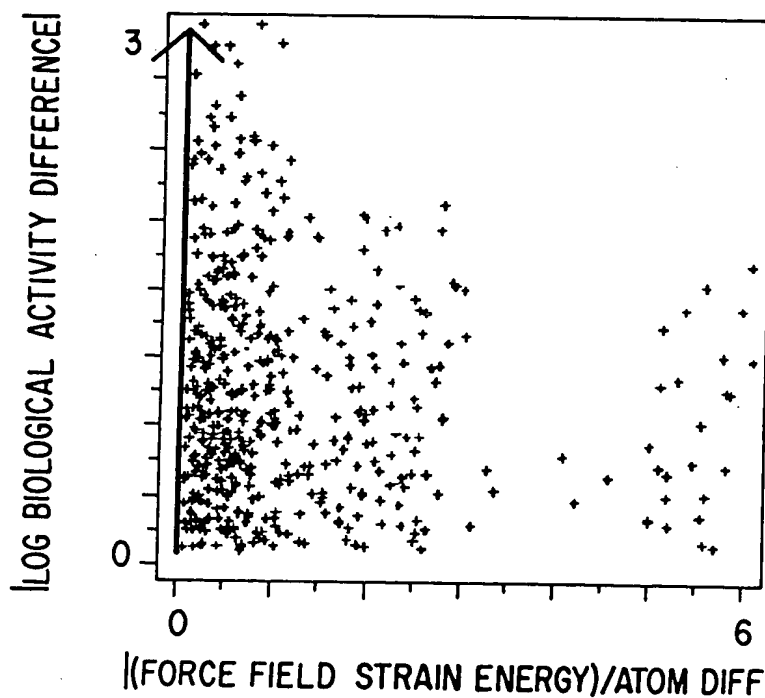


FIG. 3



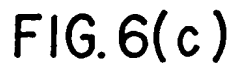
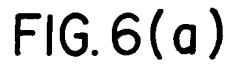
DENSITY RATIO	χ^2
1.00	0.00

FIG. 4



DENSITY RATIO	χ^2
0.96	0.46

FIG. 5



0986543.052501

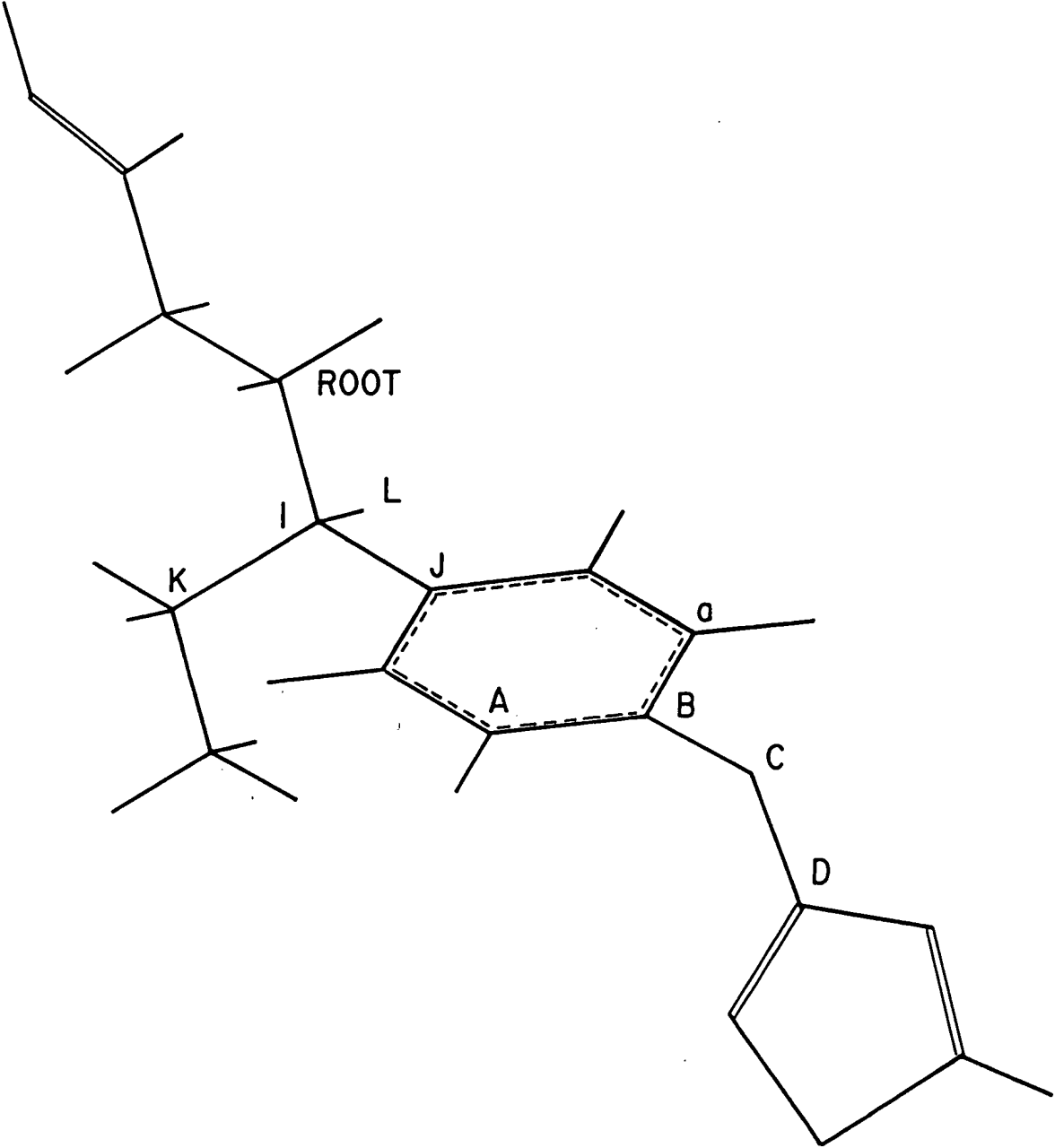


FIG. 6(d)

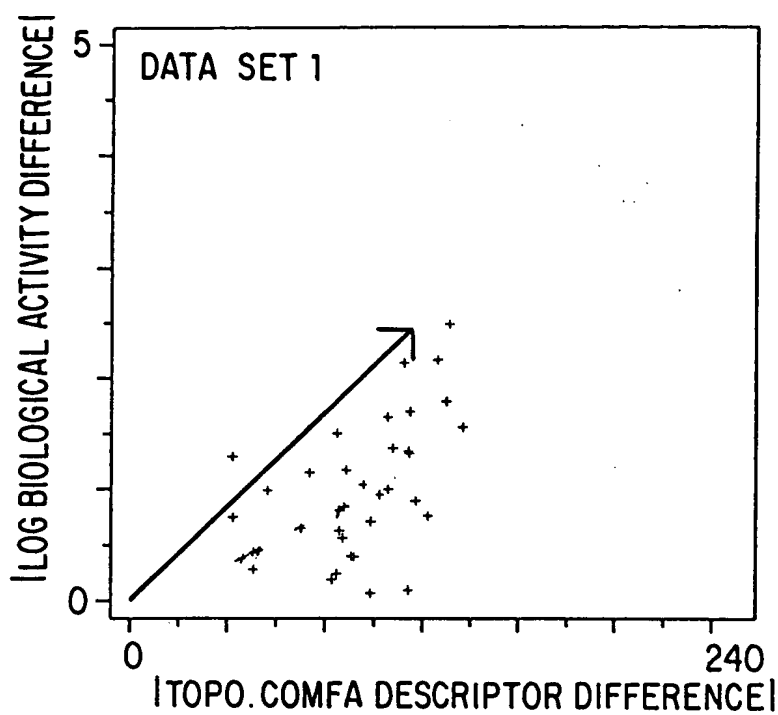


FIG.7(a)

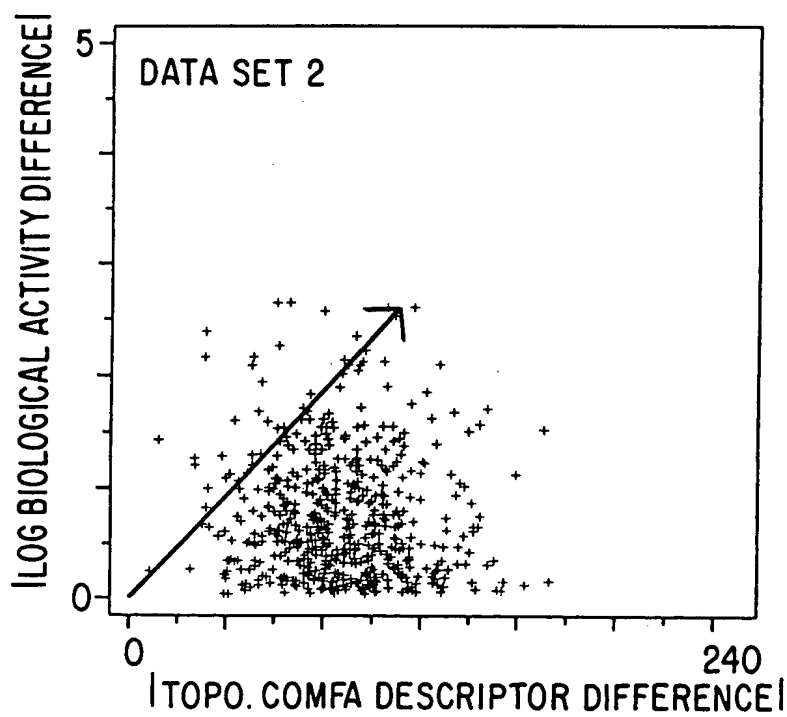


FIG.7(b)

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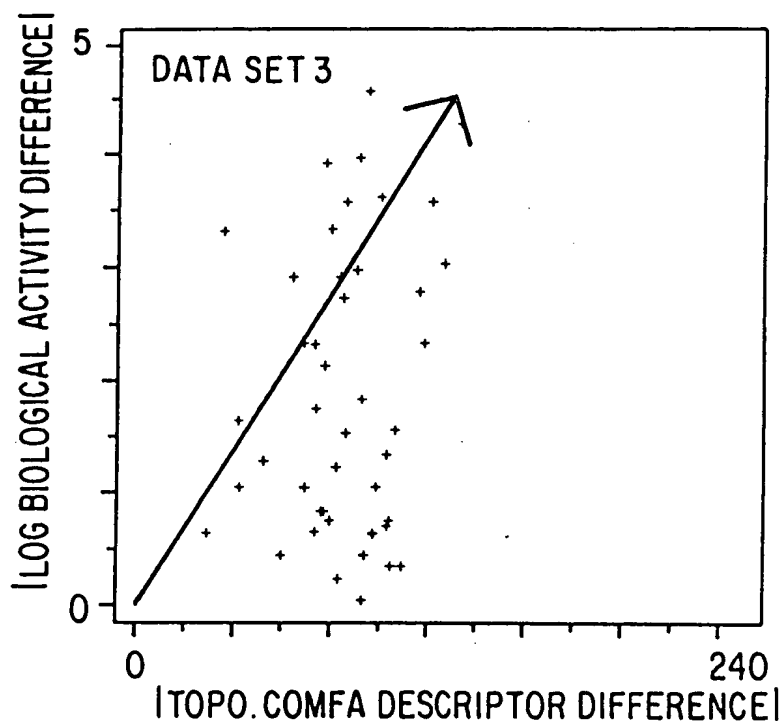


FIG. 7(c)

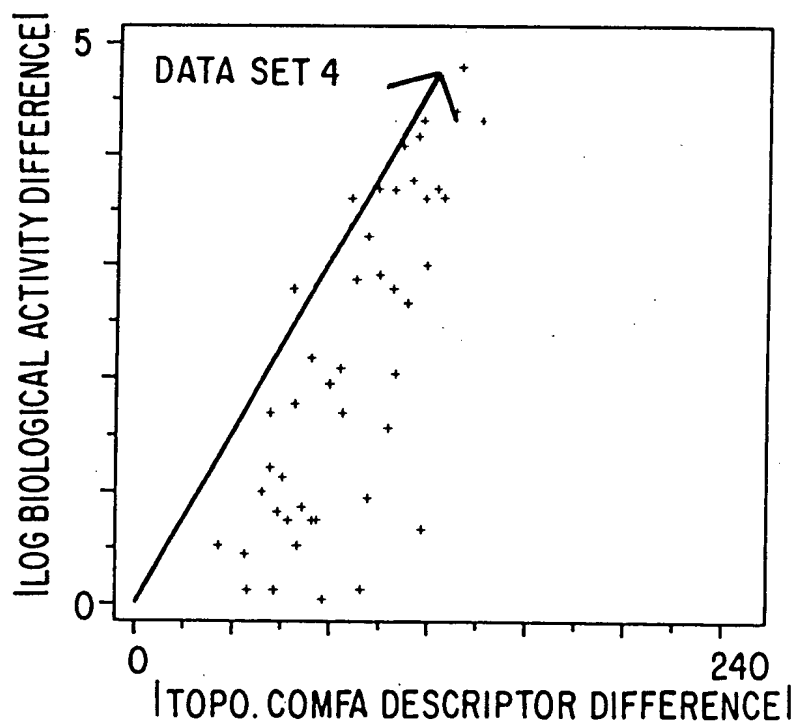


FIG. 7(d)

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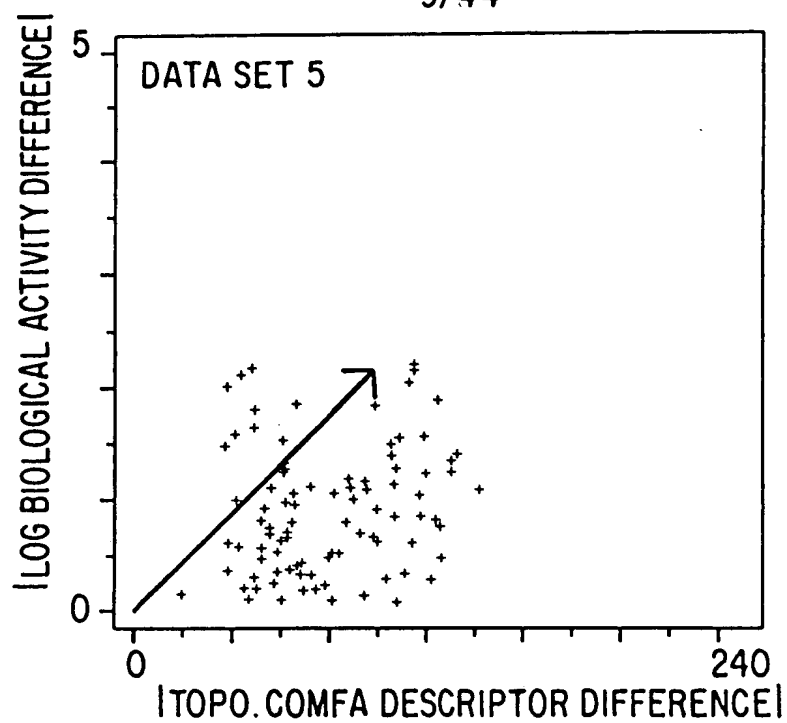


FIG.7(e)

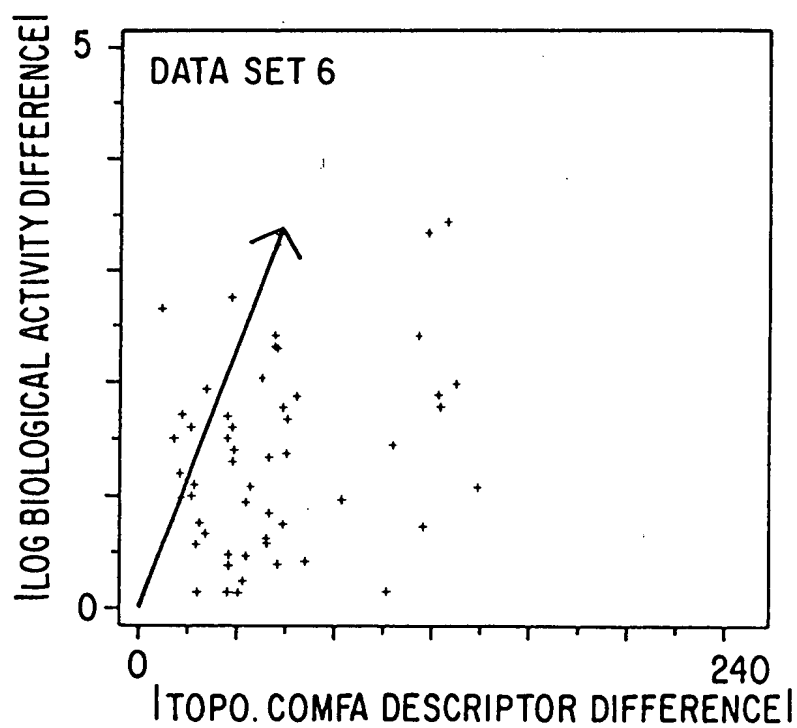
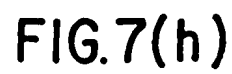
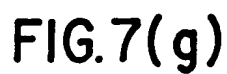


FIG.7(f)



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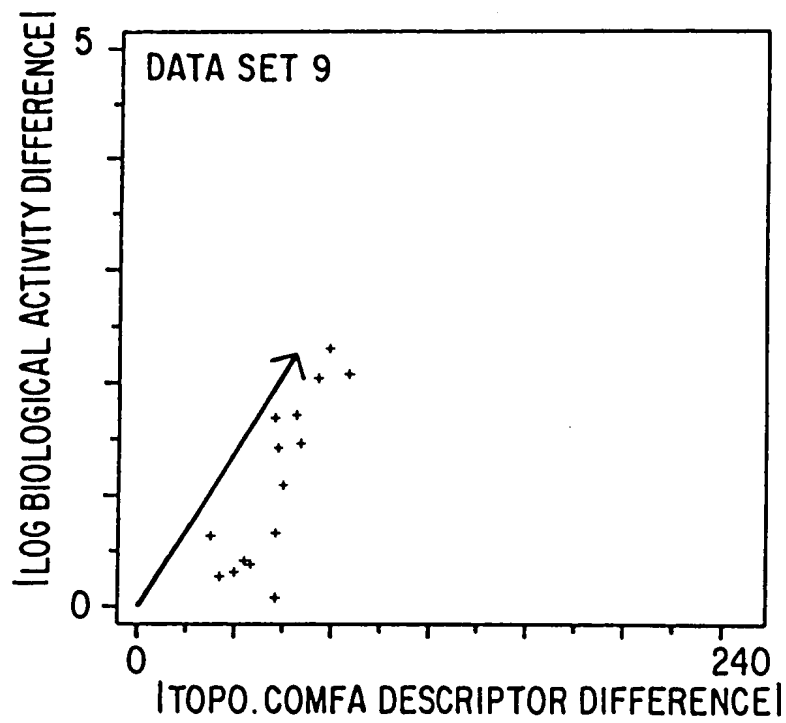


FIG.7(i)

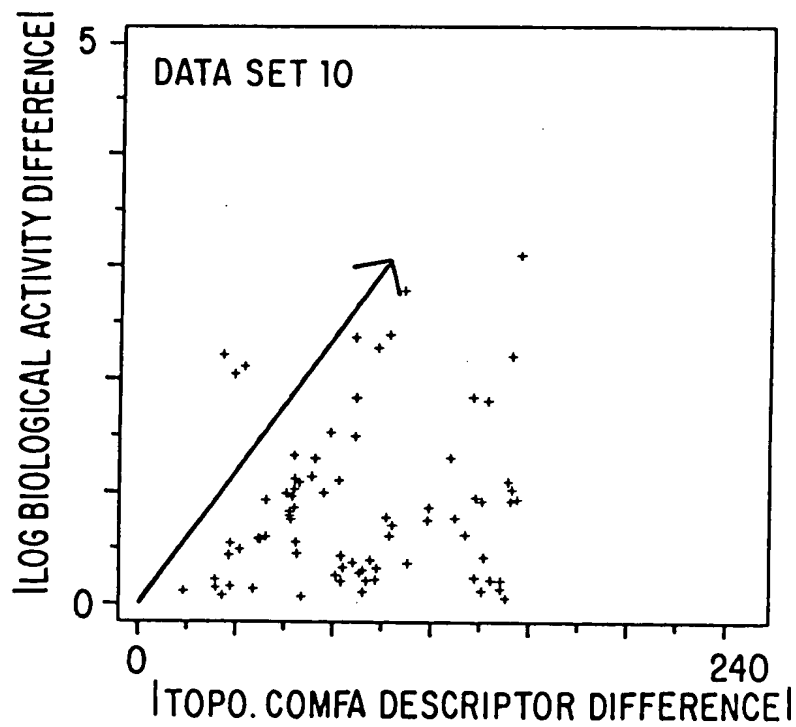


FIG.7(j)

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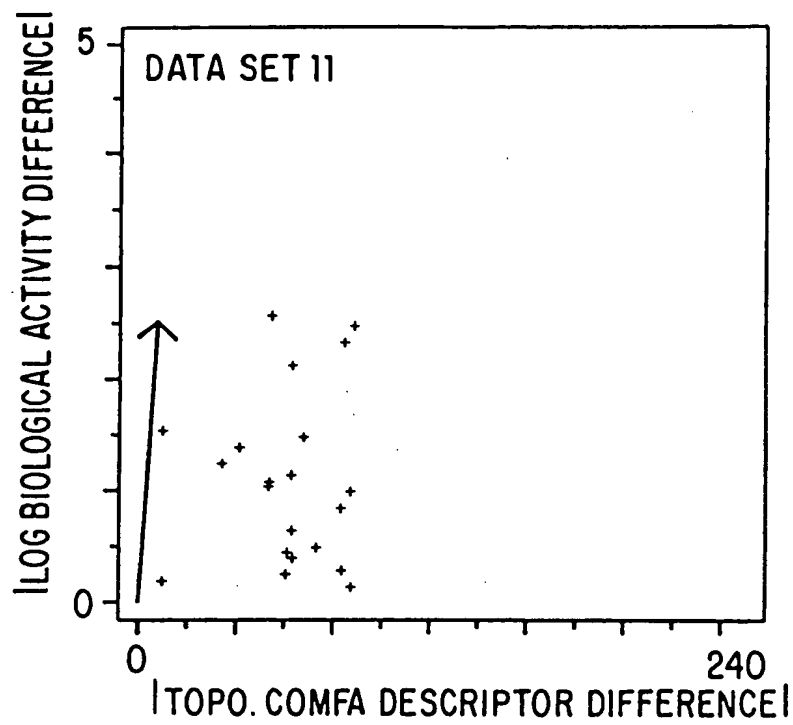


FIG.7(k)

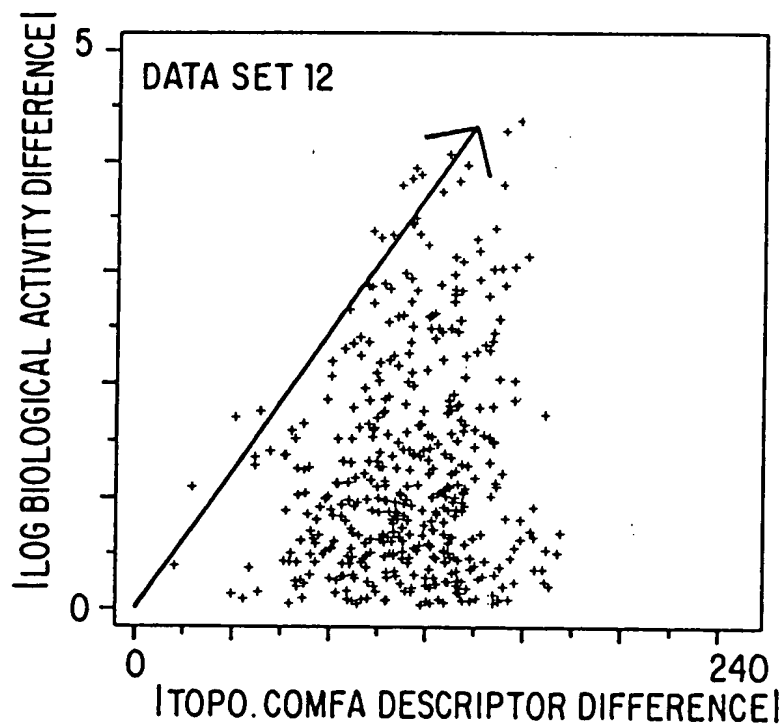


FIG.7(l)

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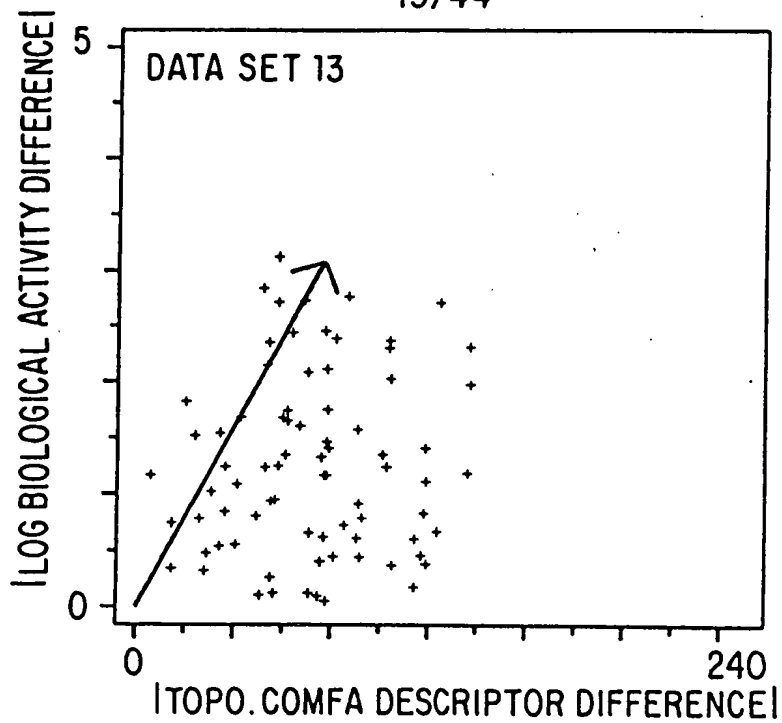


FIG.7(m)

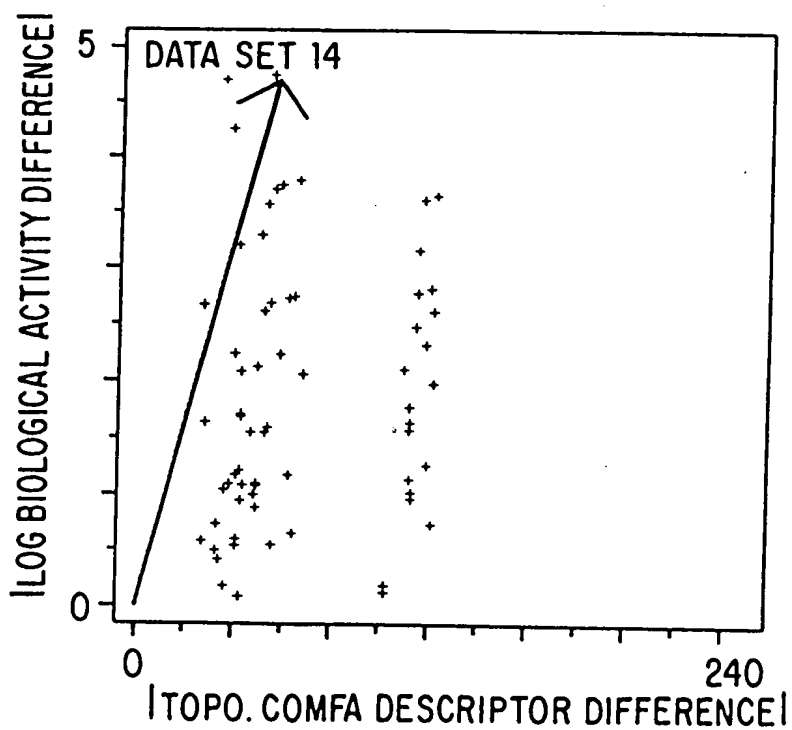


FIG.7(n)

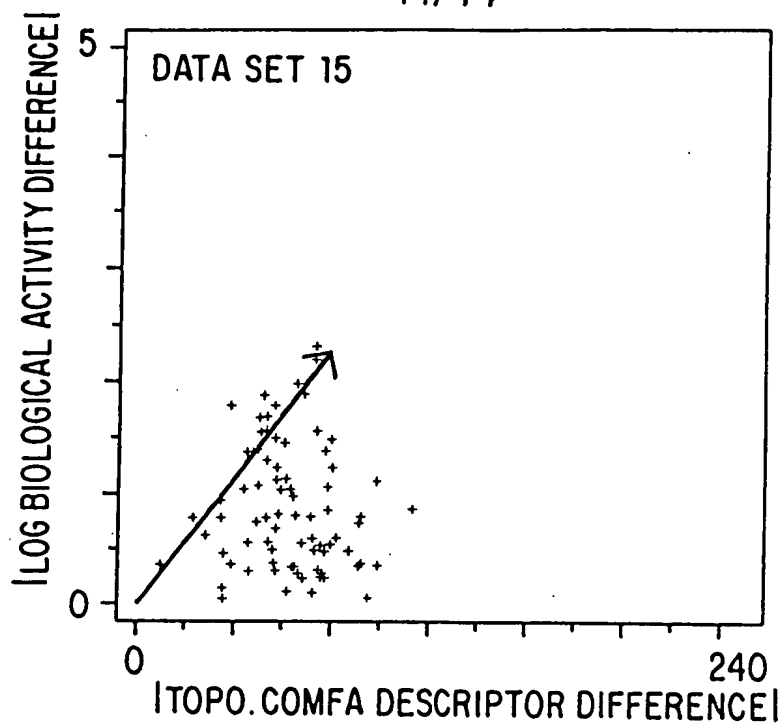


FIG. 7(o)

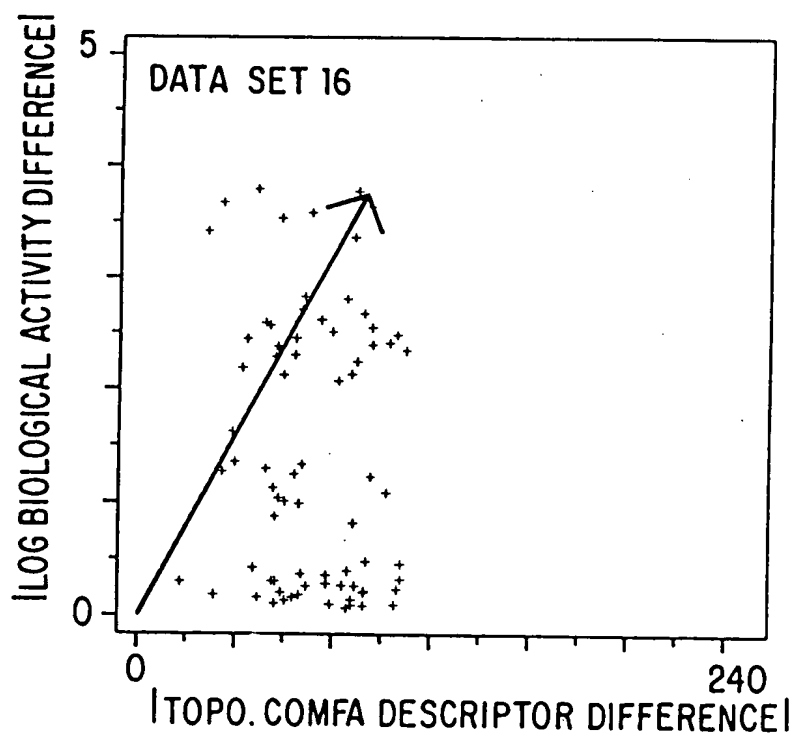


FIG. 7(p)

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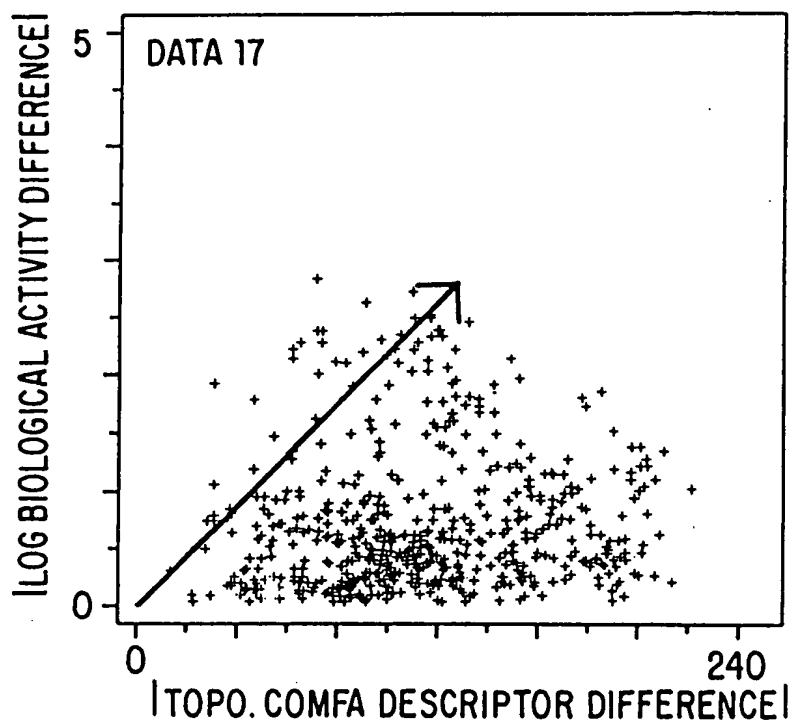


FIG.7(q)

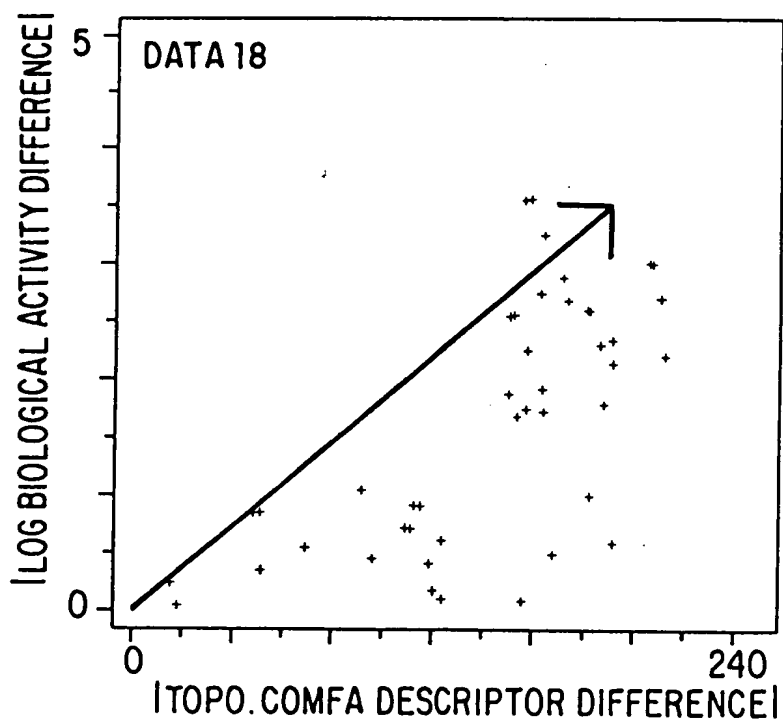


FIG.7(r)

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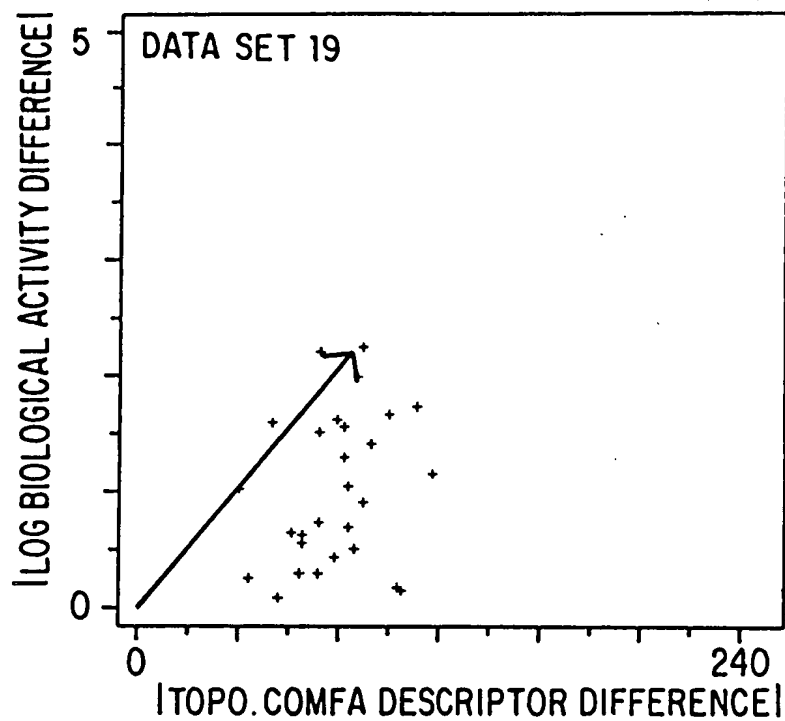


FIG. 7(s)

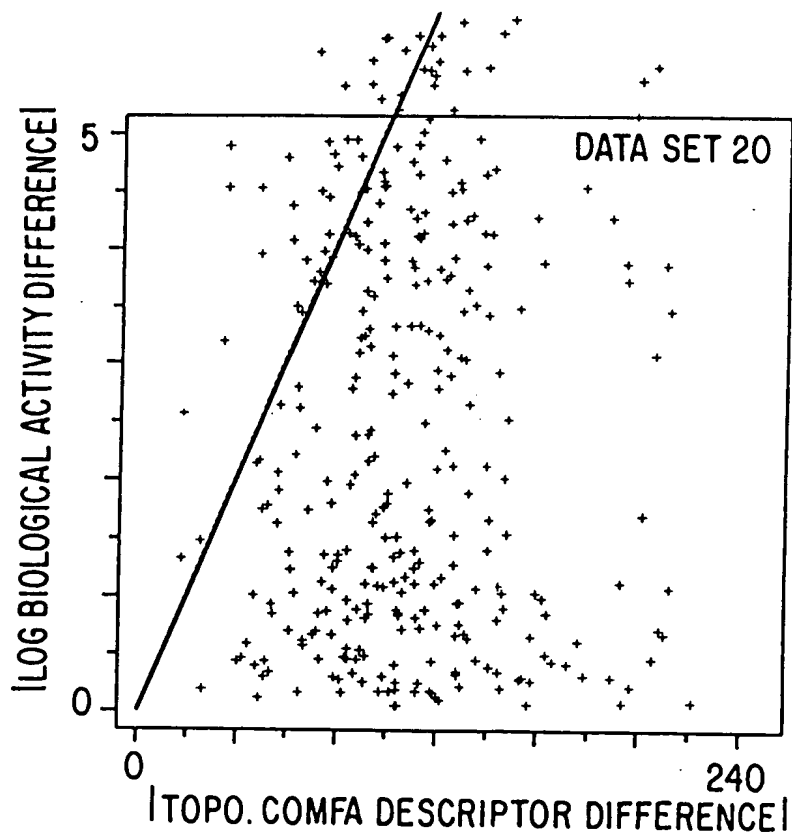
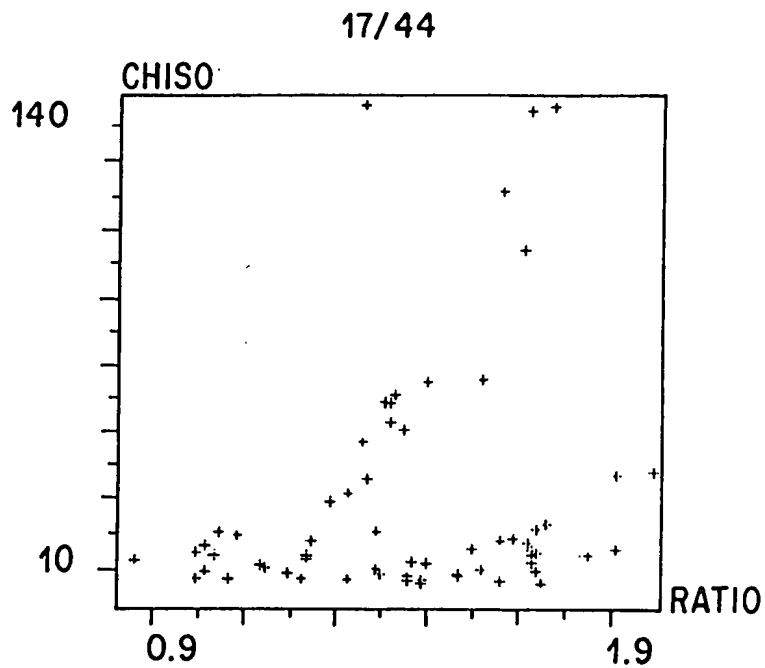


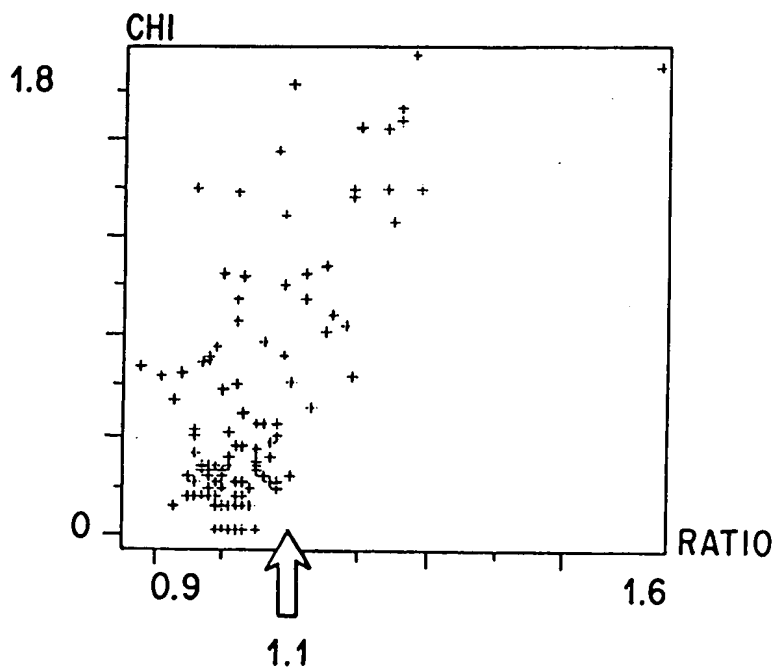
FIG. 7(t)

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T05250-24599360



1.1

FIG. 8(a)



1.1

FIG. 8(b)

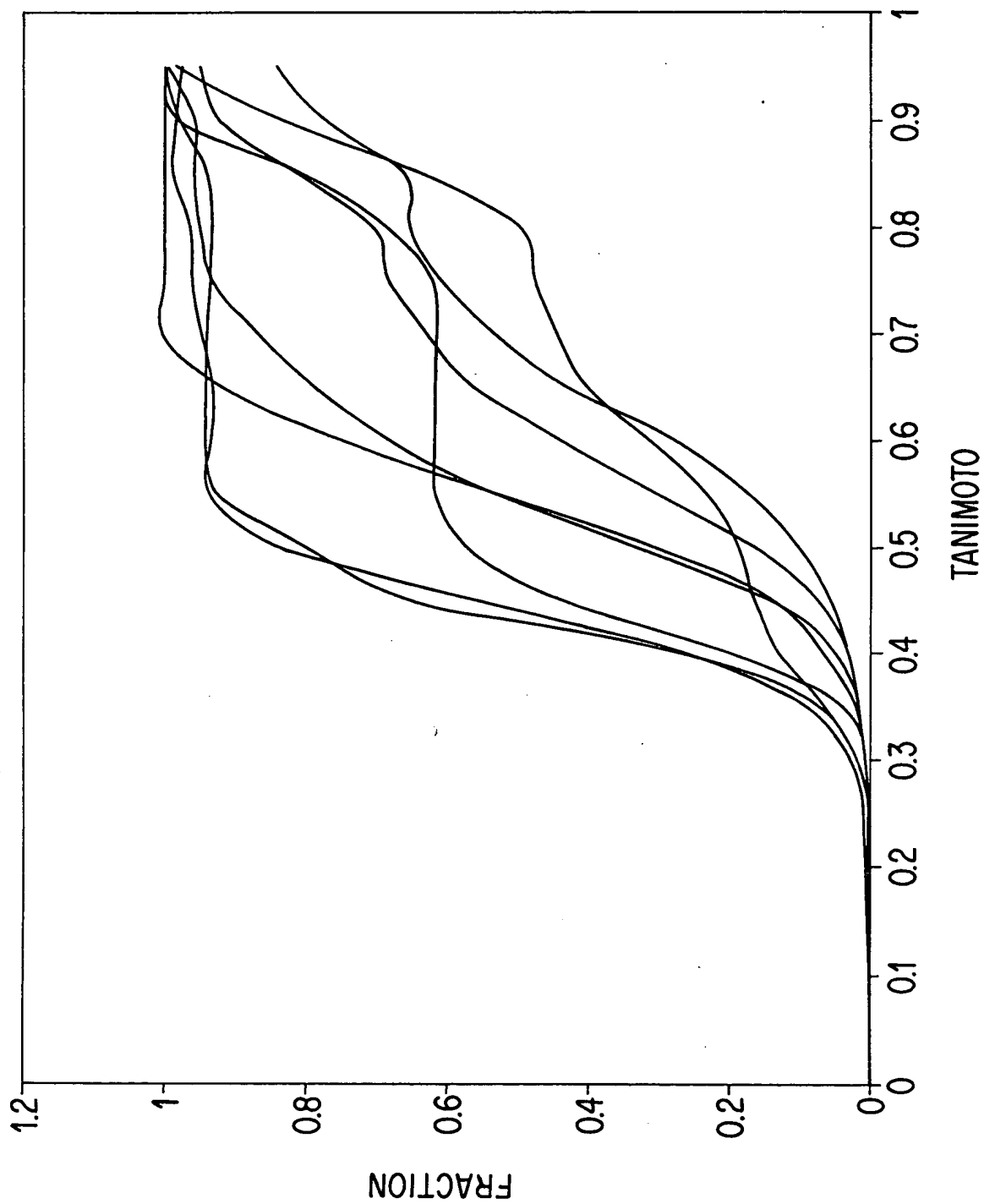


FIG. 9(a)

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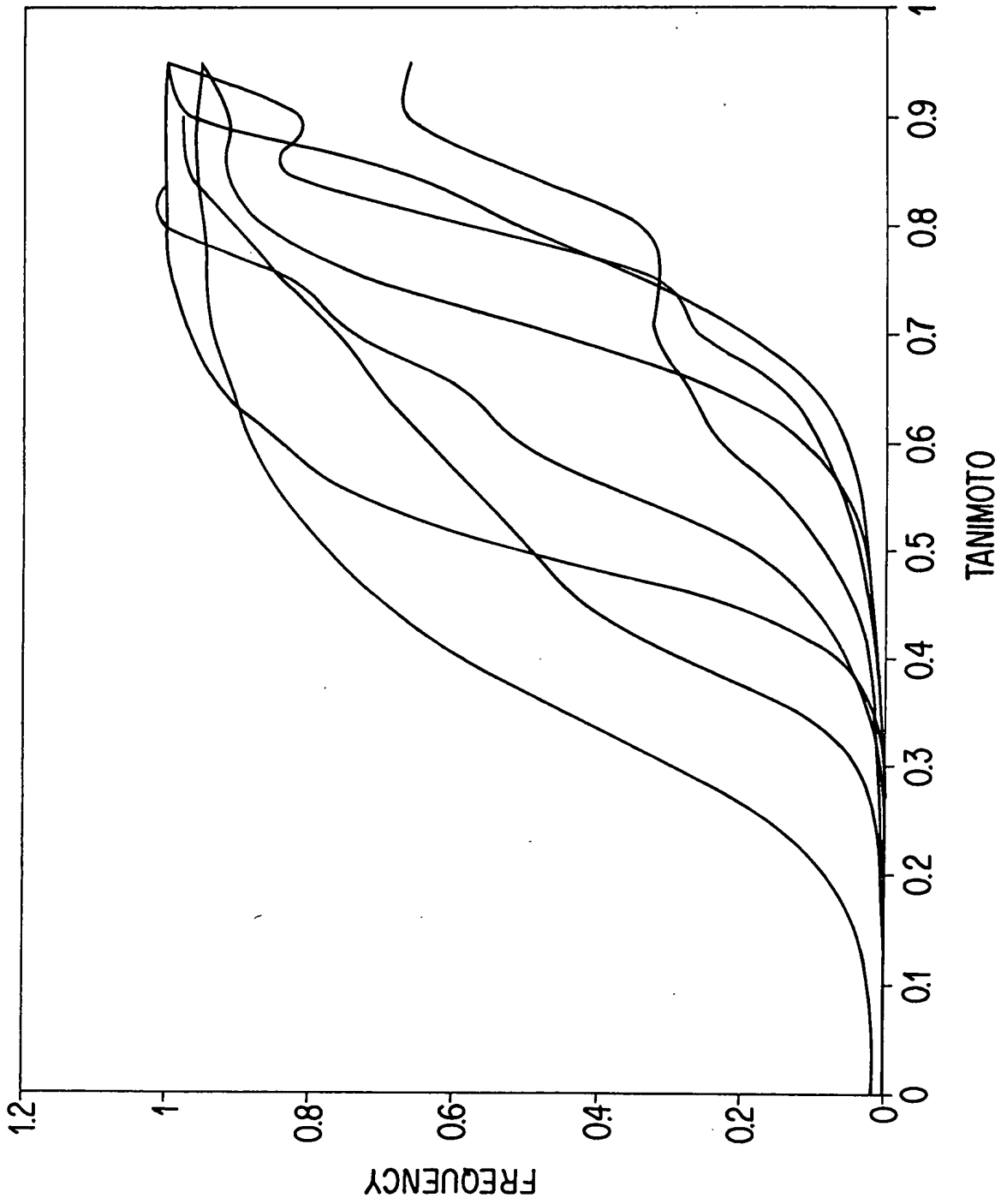
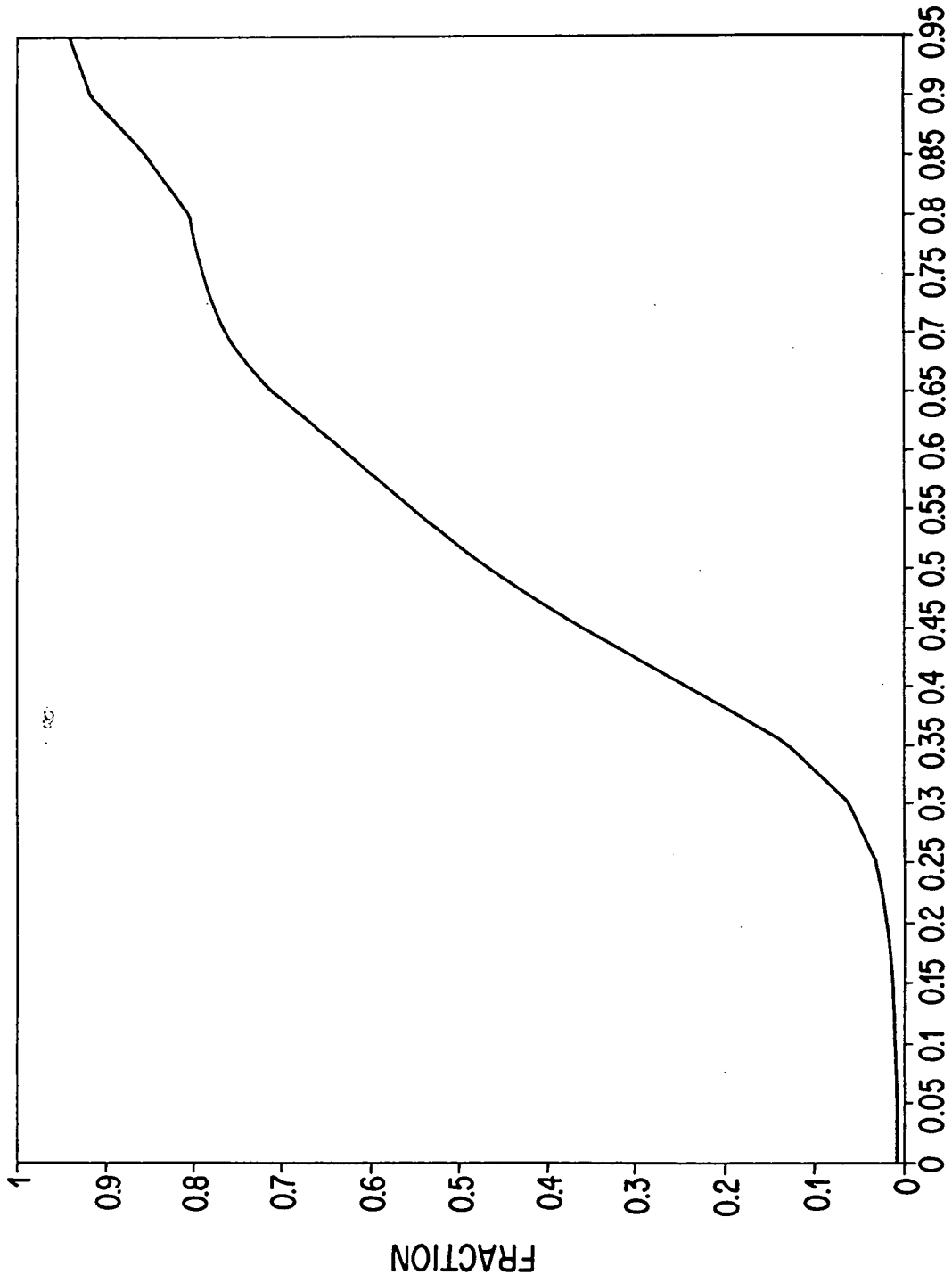


FIG. 9(b)



TANIMOTO

FIG. 9(c)

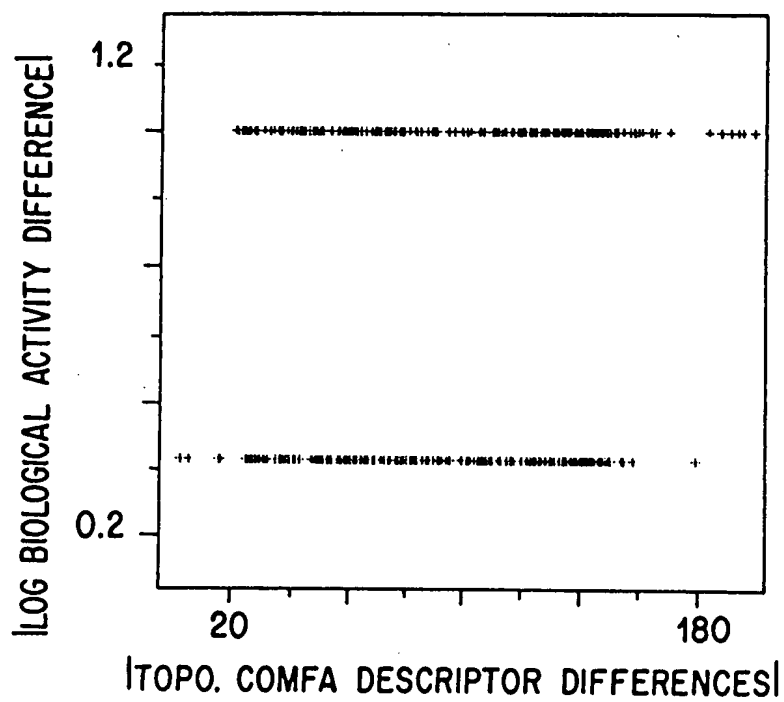


FIG.10(a)

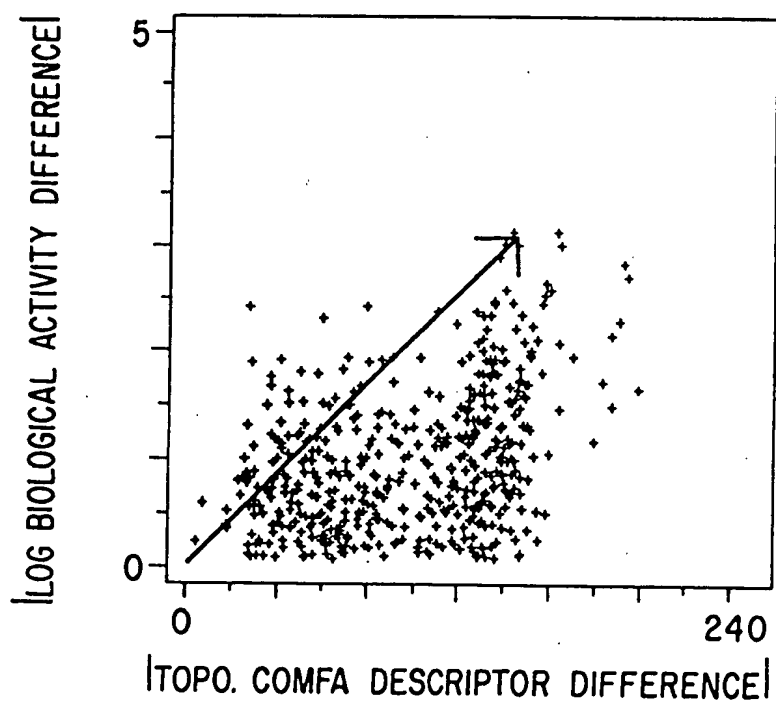


FIG.10(b)

FUNCTION

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SOFTWARE

8.

SELECT CHEMISTRY

LIST REACTANTS & CORES
DEFINE COMBINATIONS

A

2

1

ANY DATABASE OR WORD
PROCESSING PROGRAM

3

8.A

REMOVE REACTANTS:

NON-DIVERSITY REASONS



8A(i) GENERAL CRITERIA

METALS
TAUTOMERS/SALTS & COUNTER IONS
INTERFERING GROUPS
SYNTHESIS & EXTRACTION
PRICE/AVAILABILITY



B

ANY WORD PROCESSING
PROGRAM OR MOLECULAR
SPREAD SHEET (MSS)

SYBYL: SPL SCRIPTS ON
MSS INVOKING-UNITY
SEARCHES FOR
FRAGMENTS
CALCULATIONS OF MW
& CLOGP

8.(A)ii BIOLOGICAL CRITERIA:

TOXIC/METABOLICALLY
HAZARDOUS
BIOAVAILABILITY
MOLECULAR WEIGHT
CLOGP
NON-BIOLOGICALLY RELEVANT
GROUPS
SUGARS/MULTIPLE
FUNCTIONALITIES



C

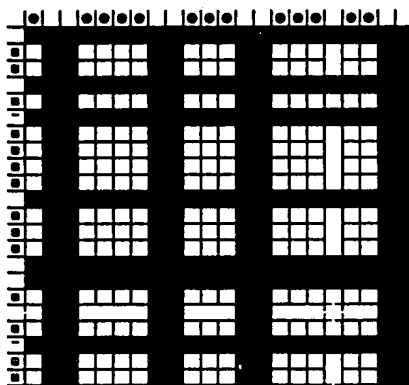
FIG.11(a)

8B

REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION
 TOPOMERIC CONFORMER
 ALIGNMENT
 CoMFA FIELD GENERATION:
 HYDROGEN BOND FIELD
 GENERATION
 ROTATABLE BOND FIELD
 ATTENUATION
 CALCULATE FIELD
 DIFFERENCES
 CLUSTER
 REACTANT SELECTION FROM
 EACH CLUSTER

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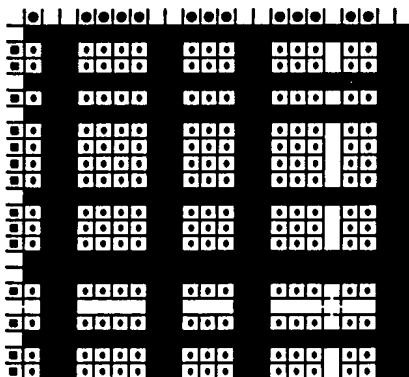
SYBYL: SELECTOR &
 CONCORD 3.2.1
 SPECIALIZED SOFTWARE:
 APPENDIX "A"
 (SYBYL: CoMFA
 STERIC & MSS)

SYBYL: HIERCHICAL
 CLUSTER - MSS
 SYLBL: MSS

8C

COMBINE REACTANTS TO BUILD PRODUCTS

E

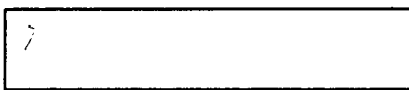


SYBYL: LEGION MSS

8D

REMOVE PRODUCTS:
NON-DIVERSITY REASONS

GENERAL CRITERIA:



SYBYL: SPL SCRIPTS
 ON MSS

F

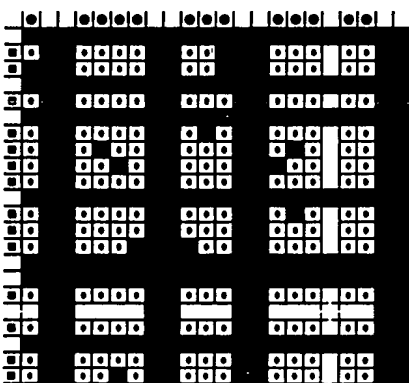


FIG.11(b)

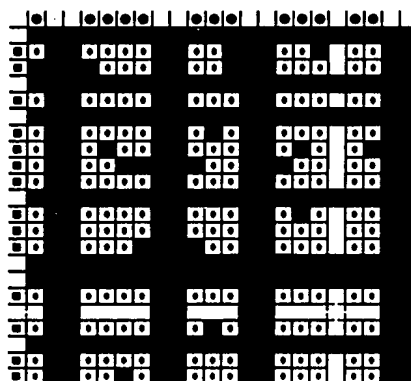
T05250" 04599860

8D

BIOLOGICAL CRITERIA:
 METABOLICALLY HAZARDOUS
 BIOAVAILABILITY
 MOLECULAR WEIGHT
 CLOGP

SYBYL: SPL SCRIPTS ON
 MSS INVOKING -
 UNITY SEARCHES FOR
 FRAGMENTS
 CALCULATIONS OF MW
 & CLOGP

G



8E

REMOVE NON-DIVERSE
PRODUCTS:

GENERATE TANIMOTO
 2D FINGERPRINTS
 SAMPLE PRODUCTS:
 EXCLUDE TAN ≥ 0.85

UNITY

H

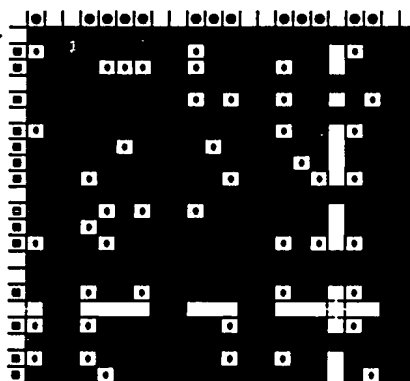
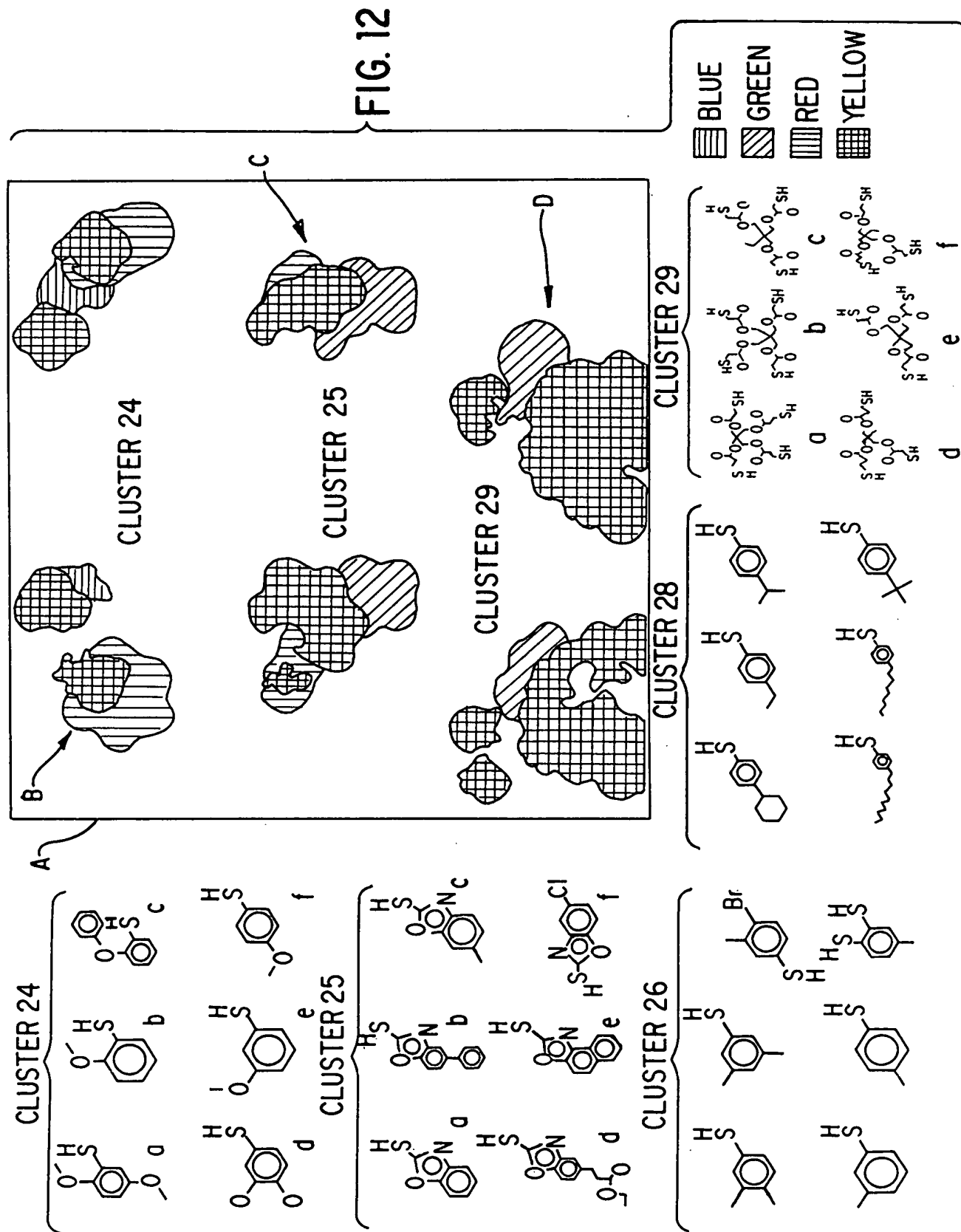


FIG.11(c)



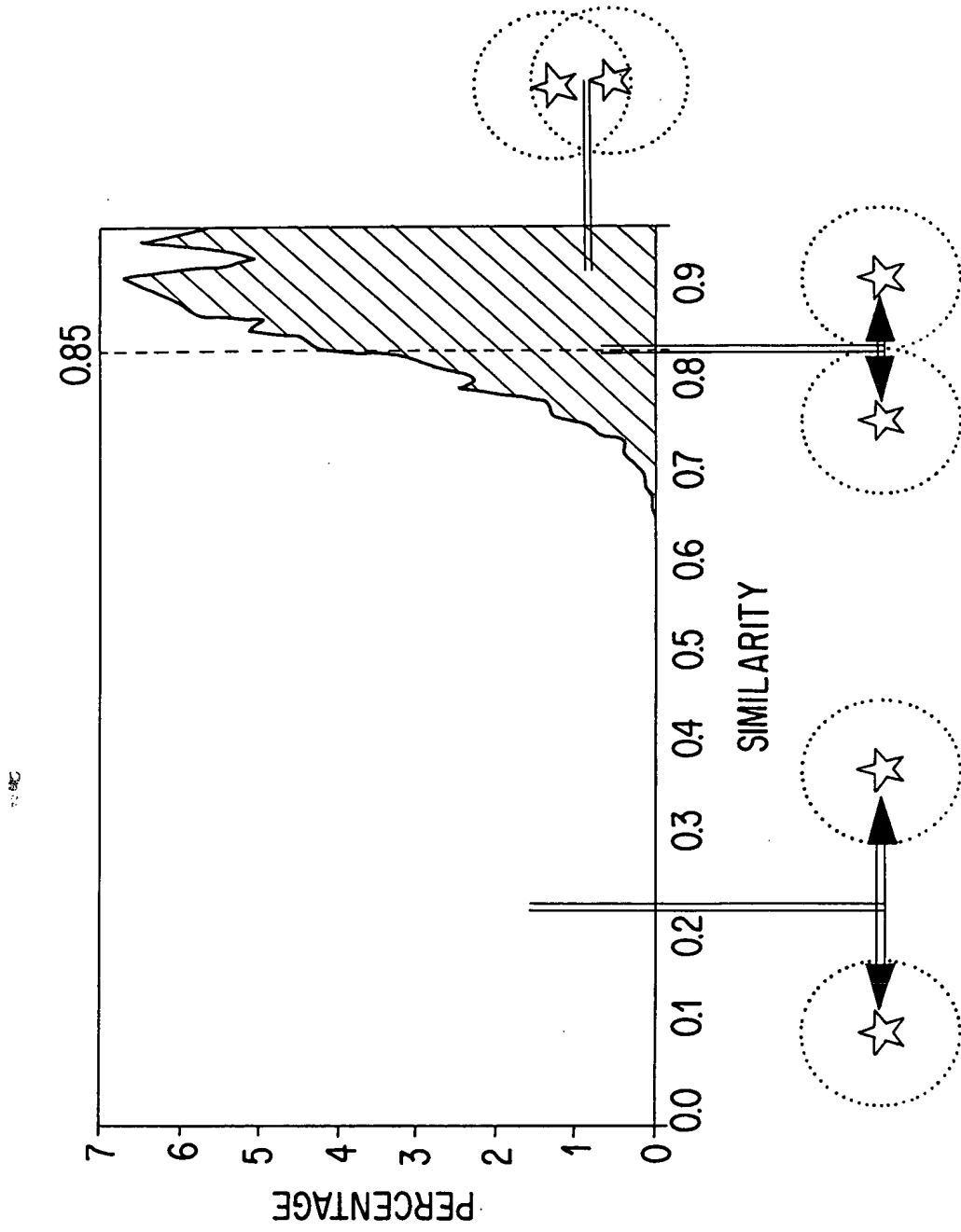


FIG. 13

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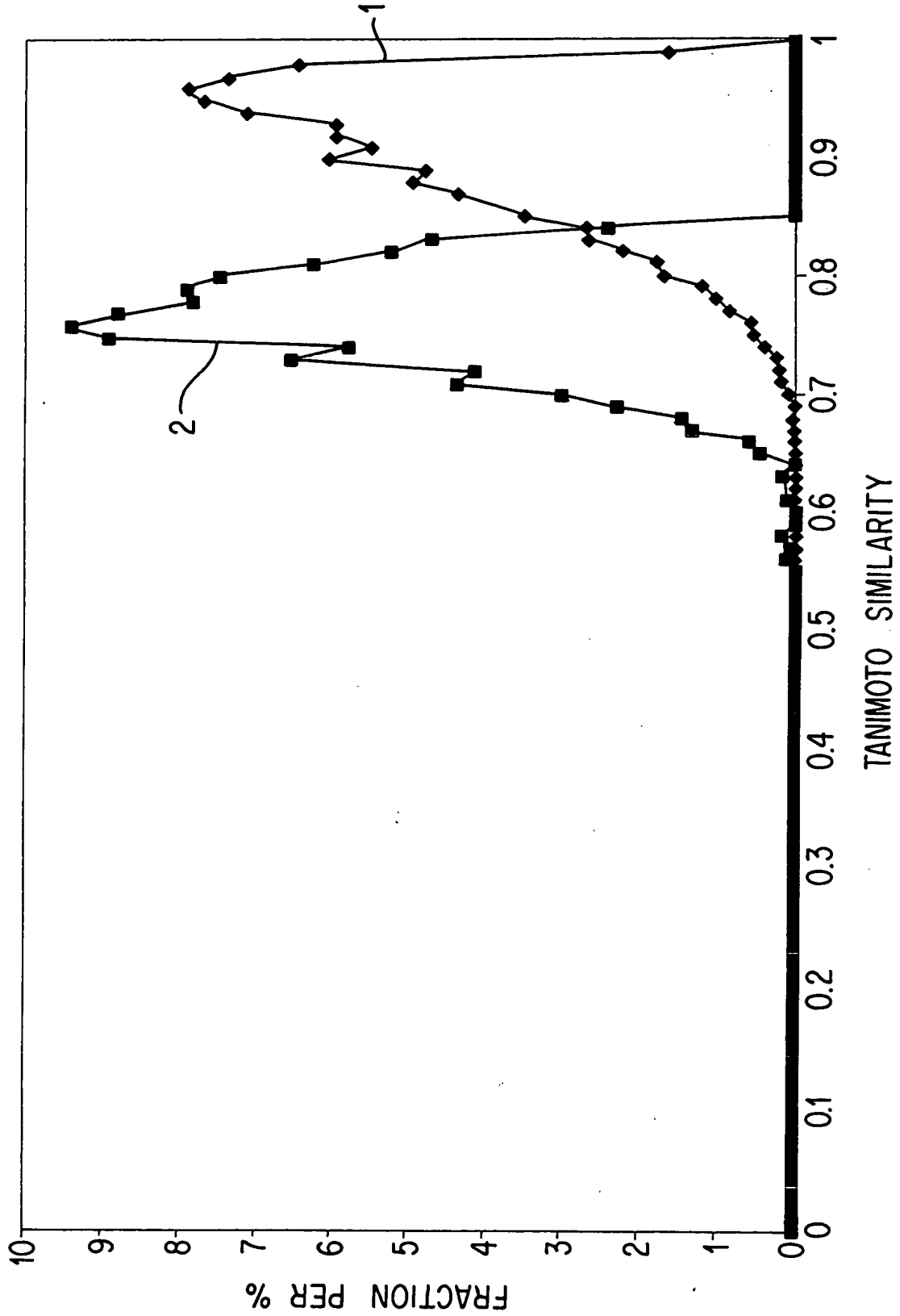
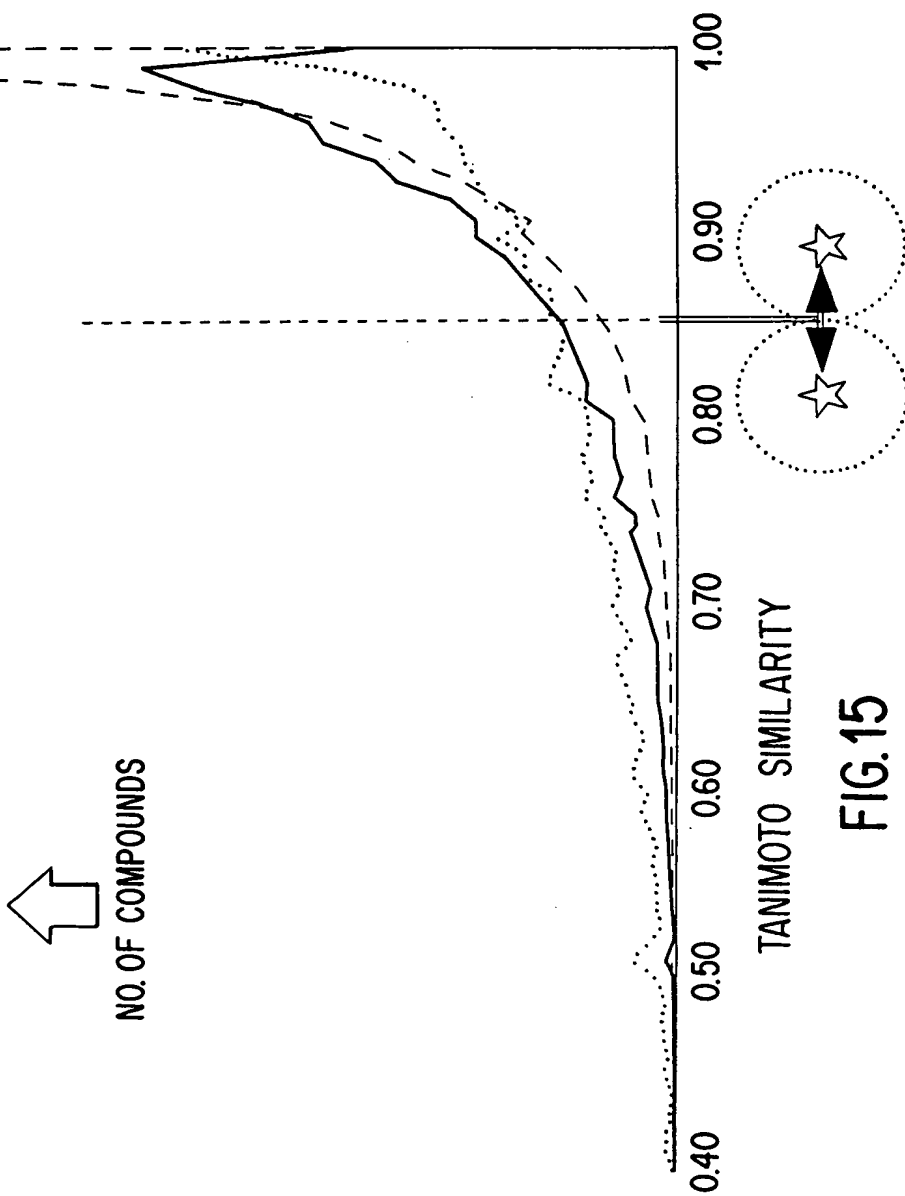


FIG.14



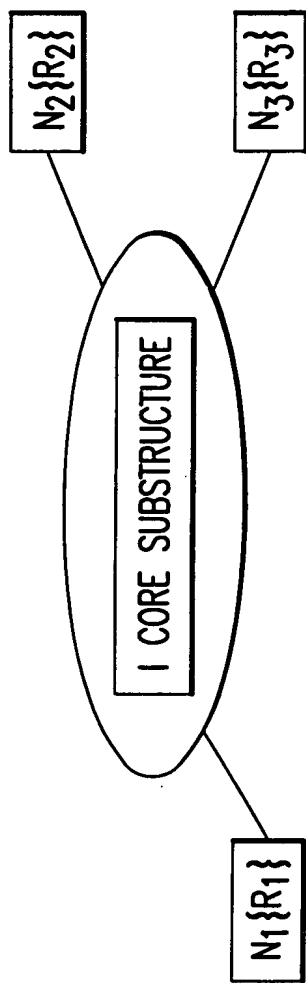


FIG.16

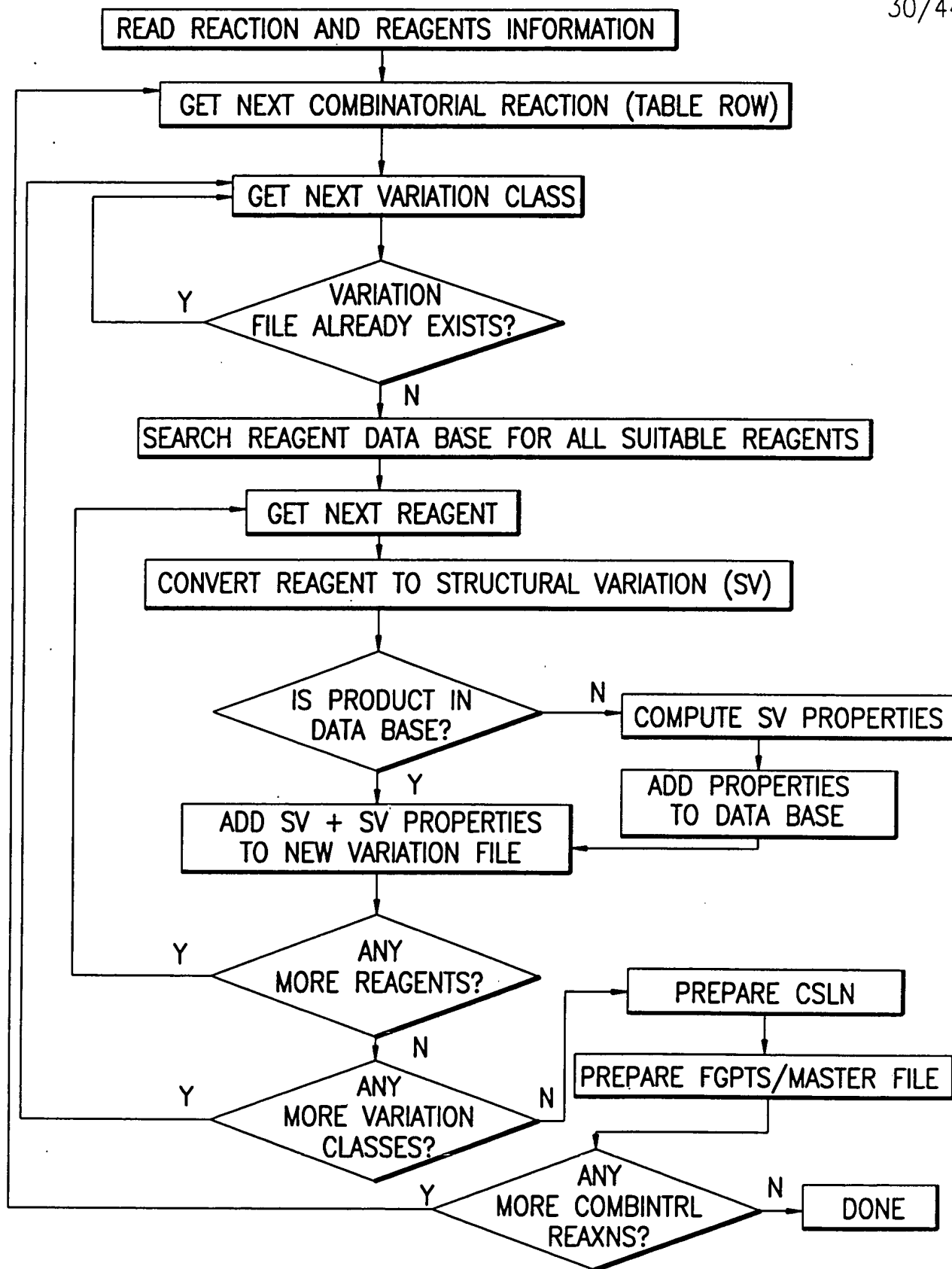


FIG.17

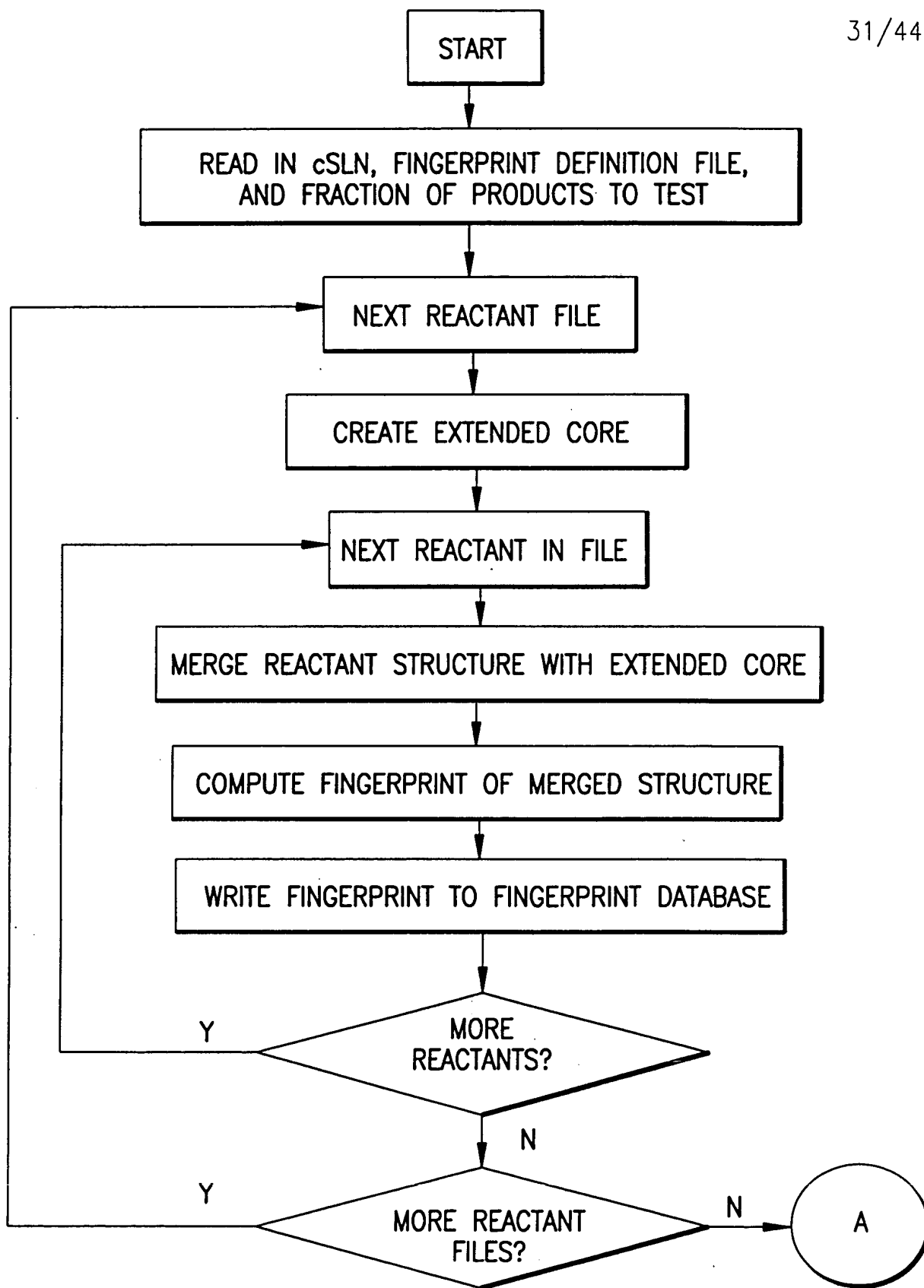


FIG.18

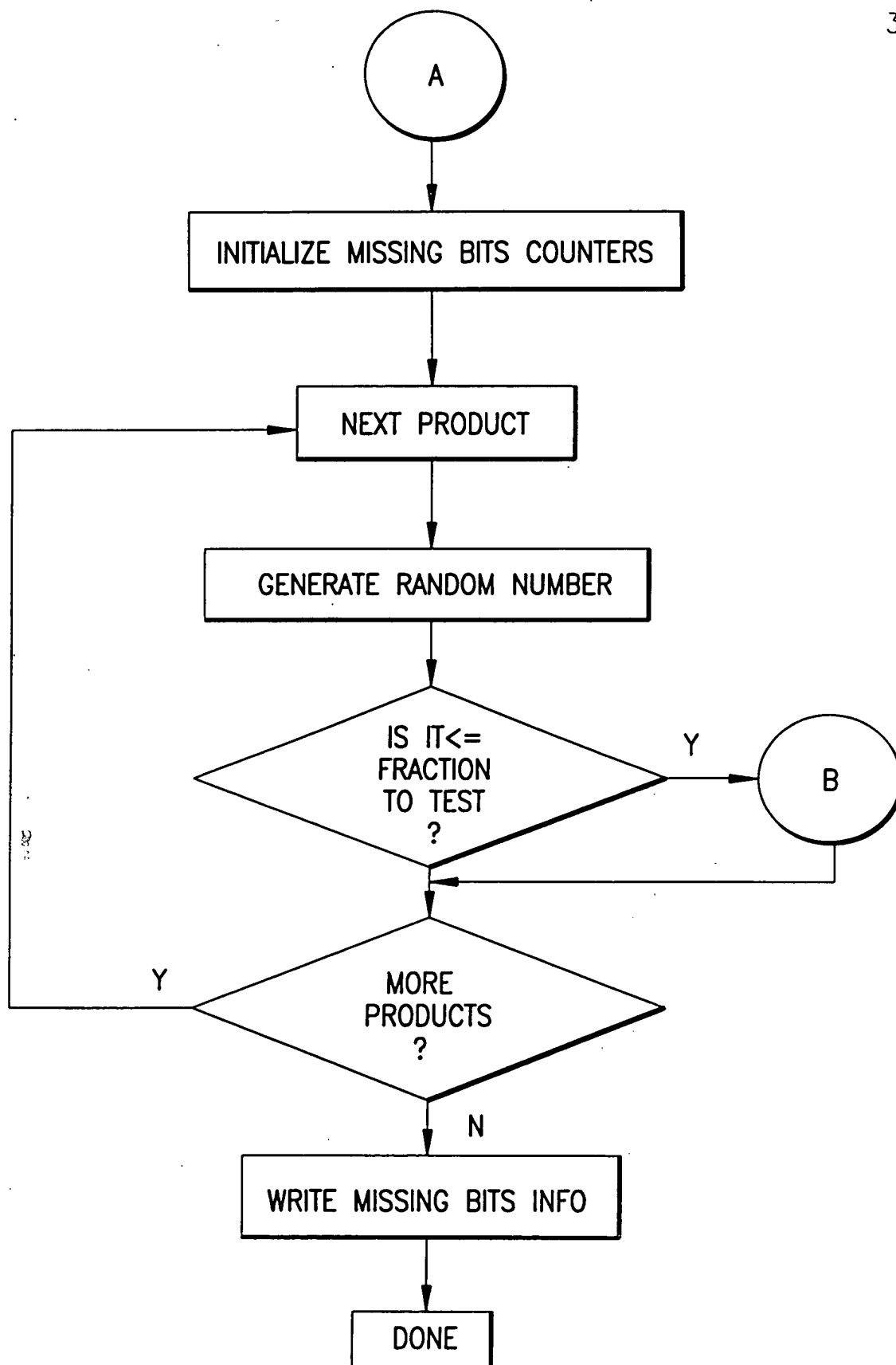


FIG.19

T05250" 052501

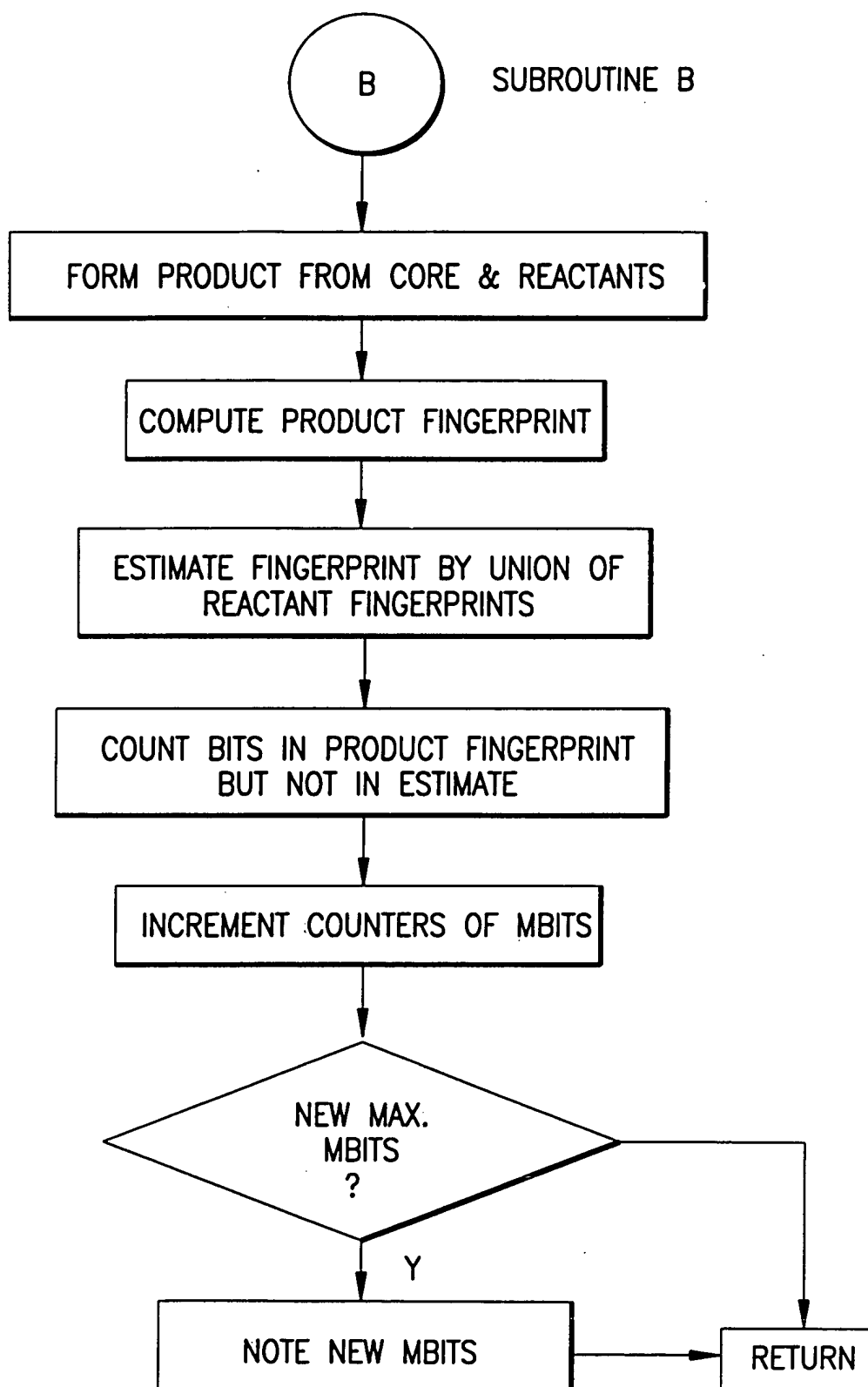


FIG.20

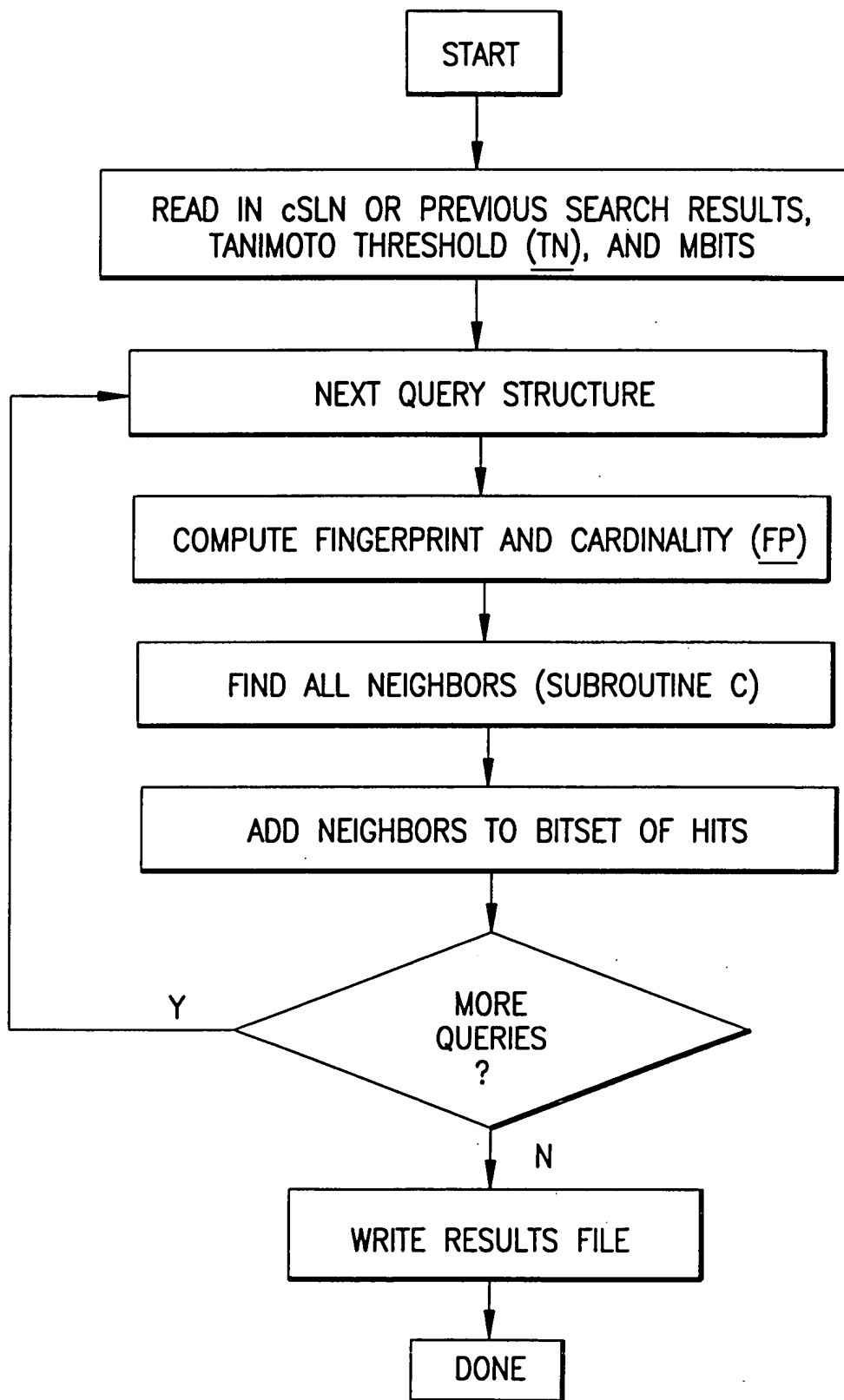
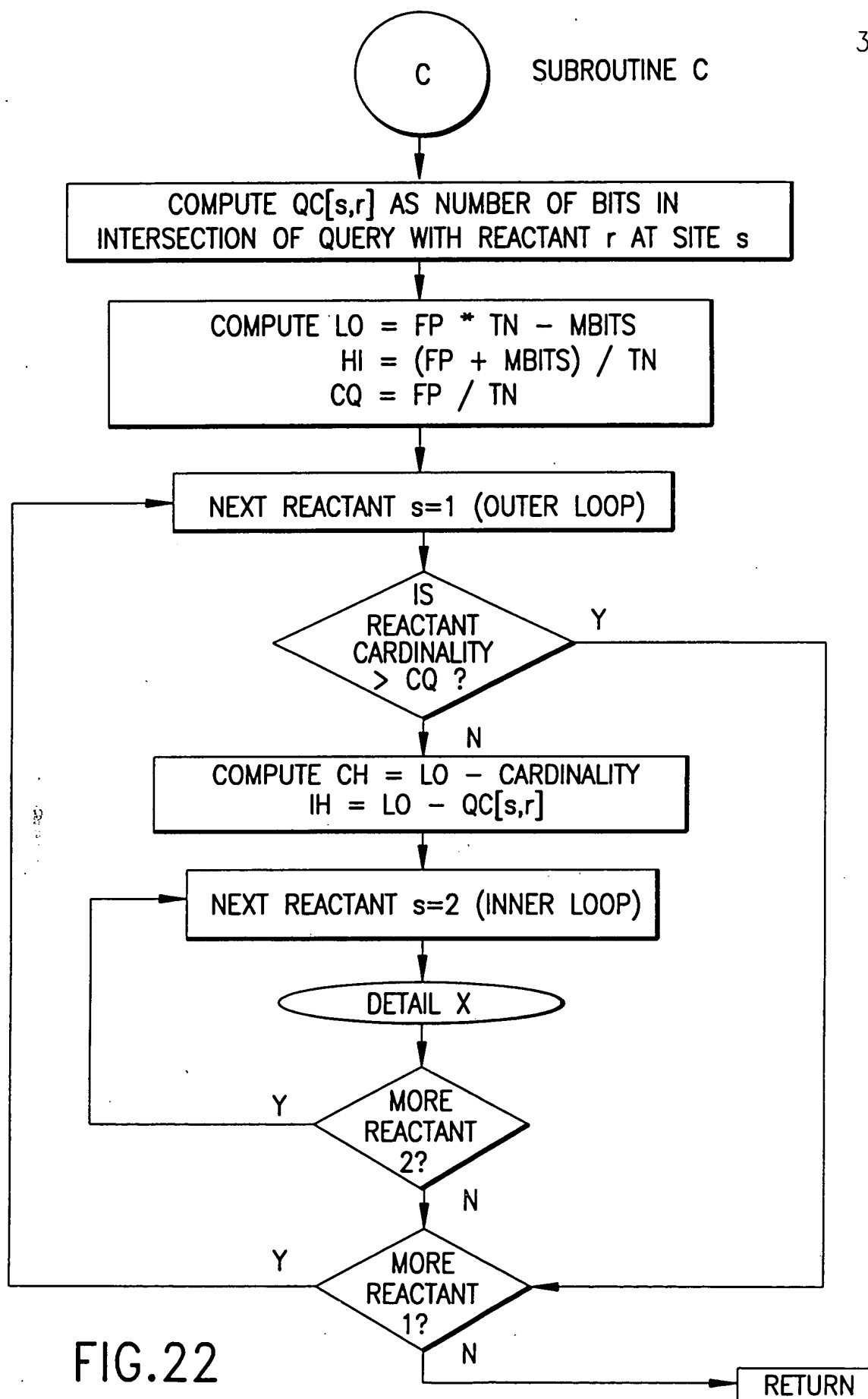


FIG.21



09664-0500 4550" 4550" 4550"

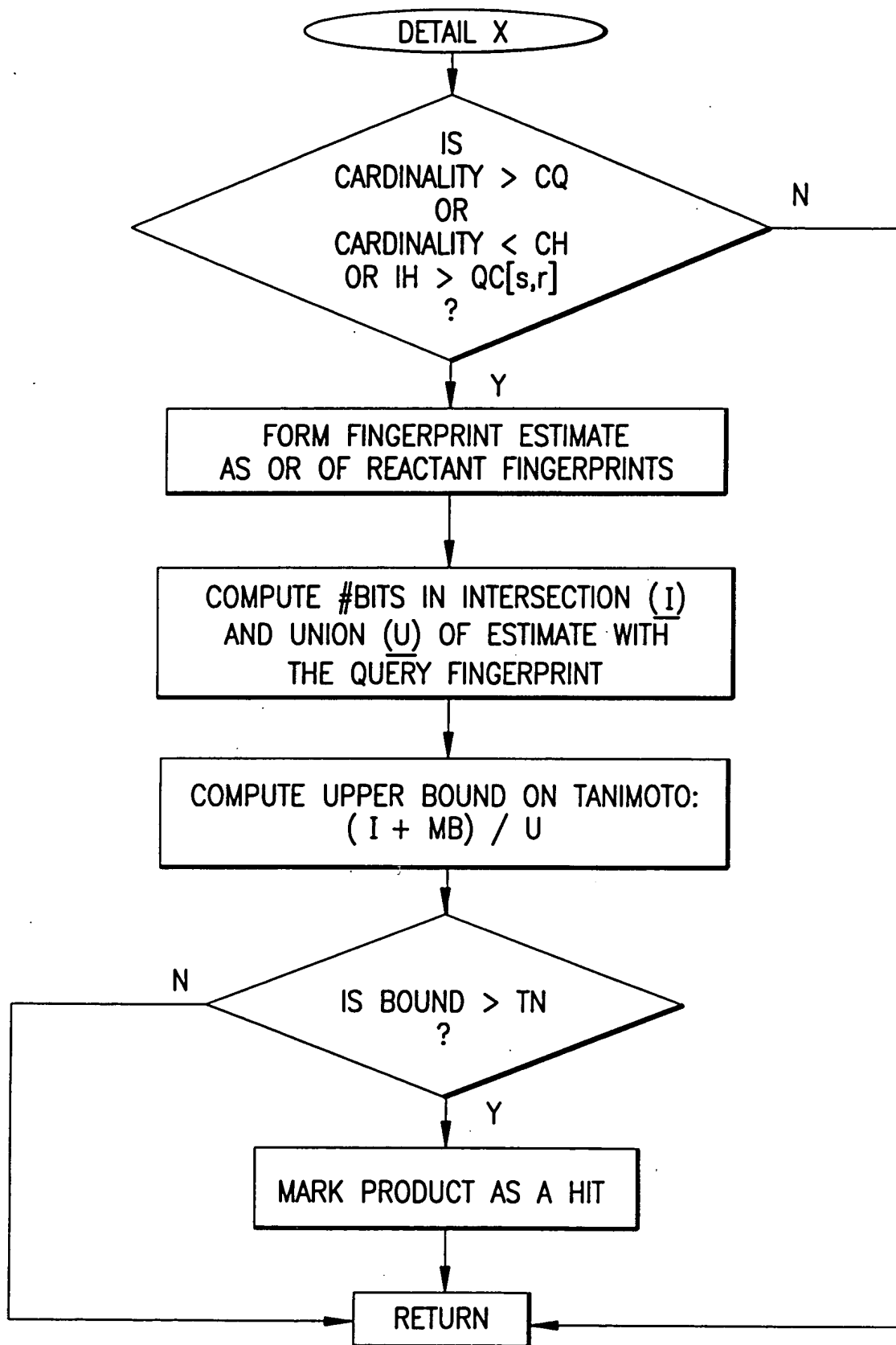


FIG.23

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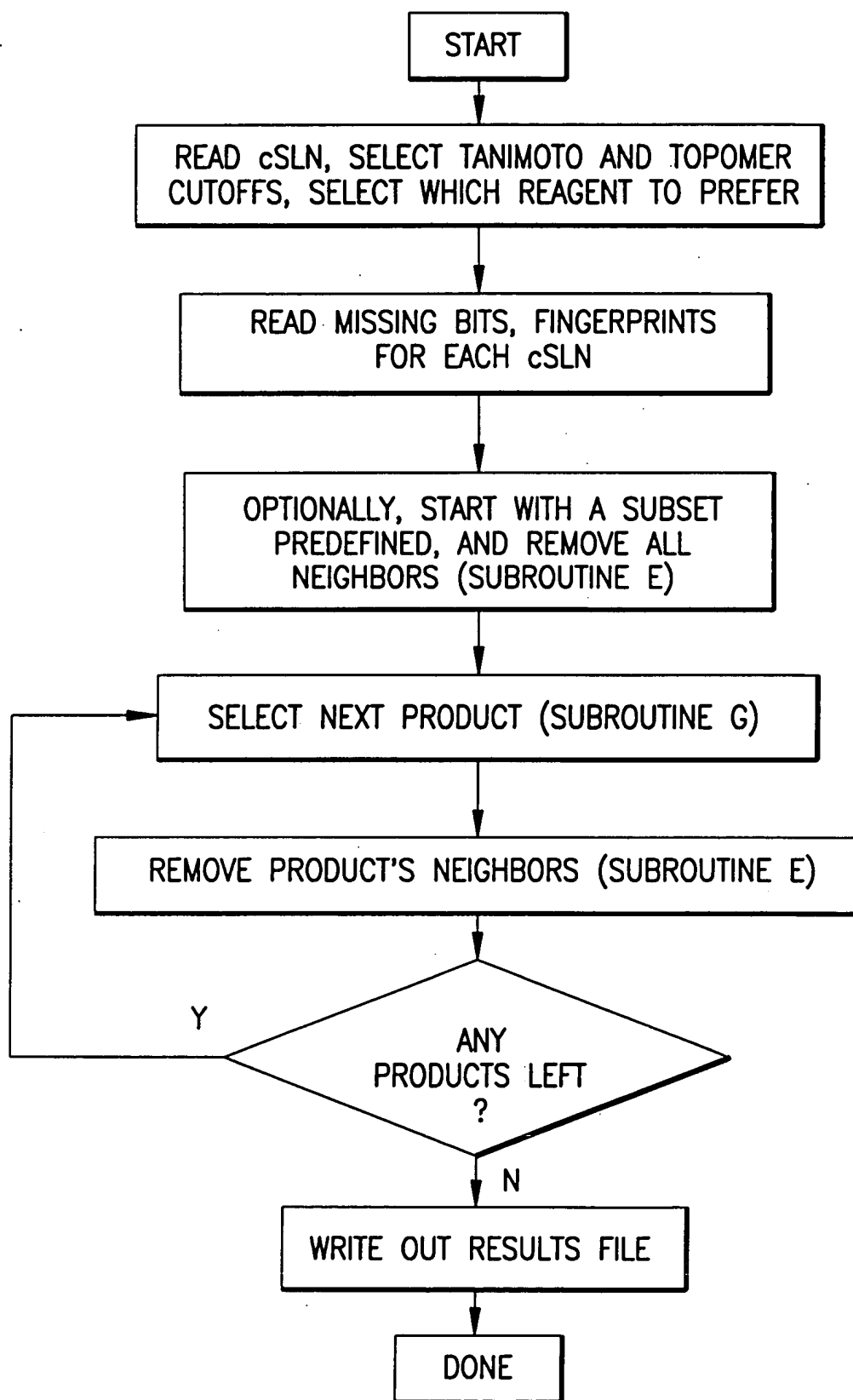


FIG.24

09664-0520
T0250-CH59260

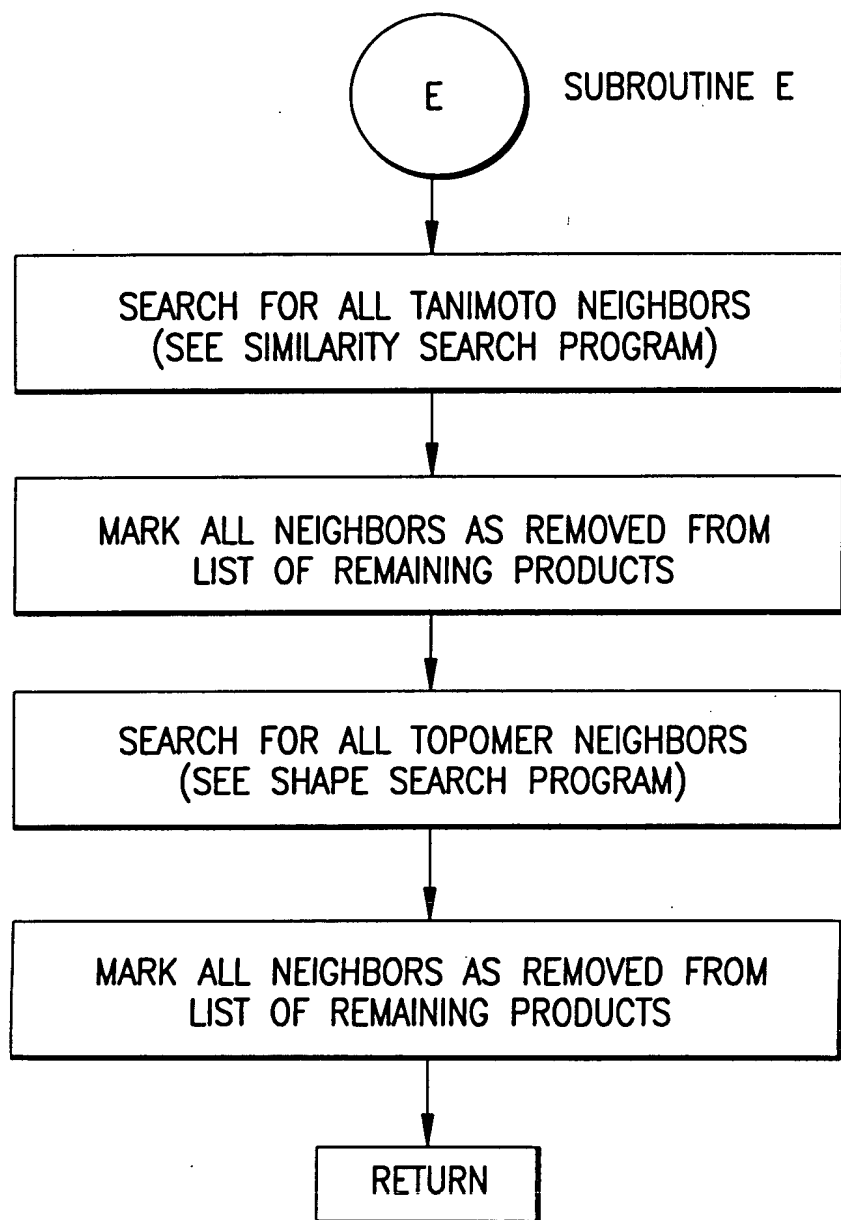


FIG.25



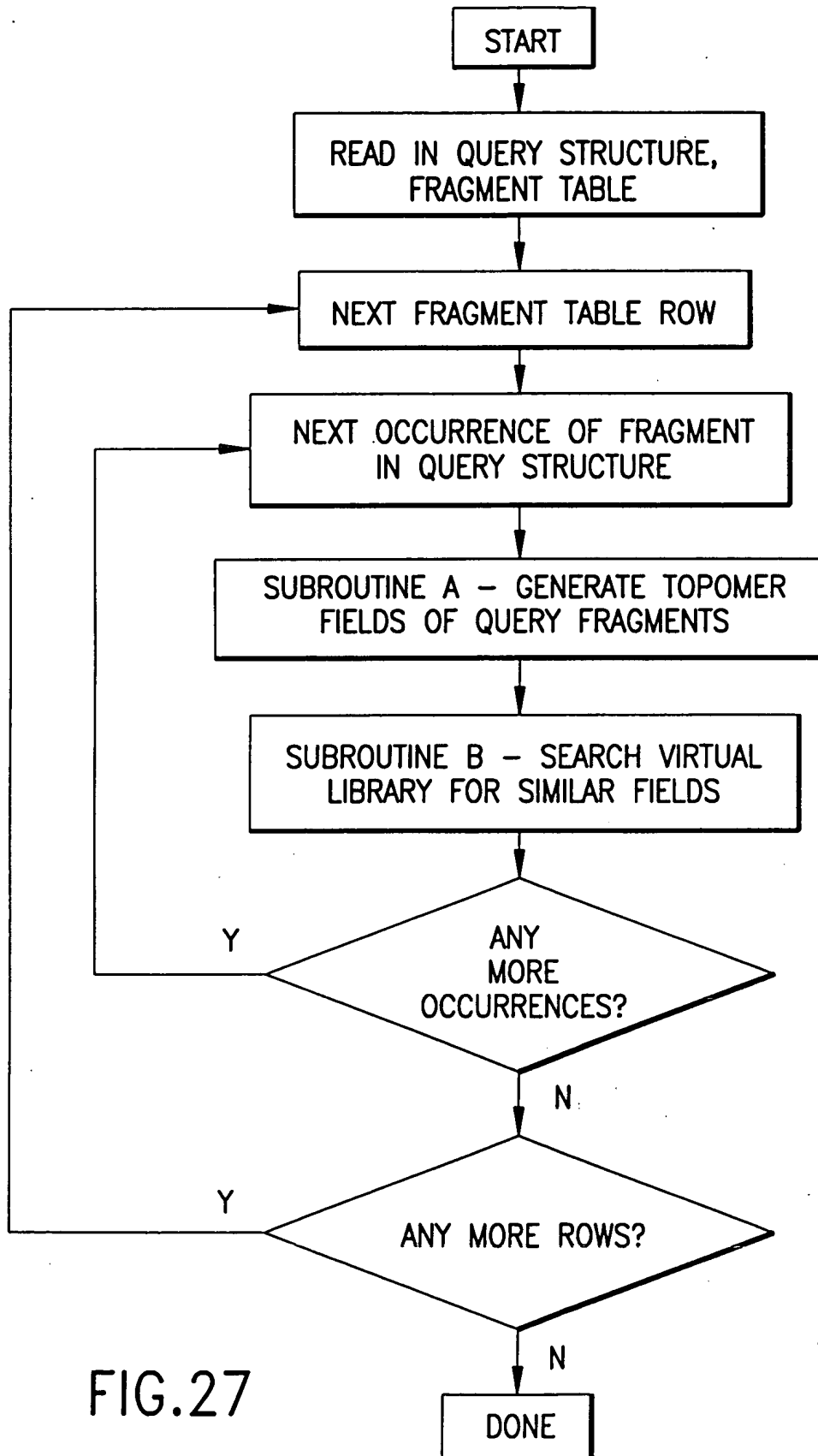


FIG.27

SUBROUTINE A

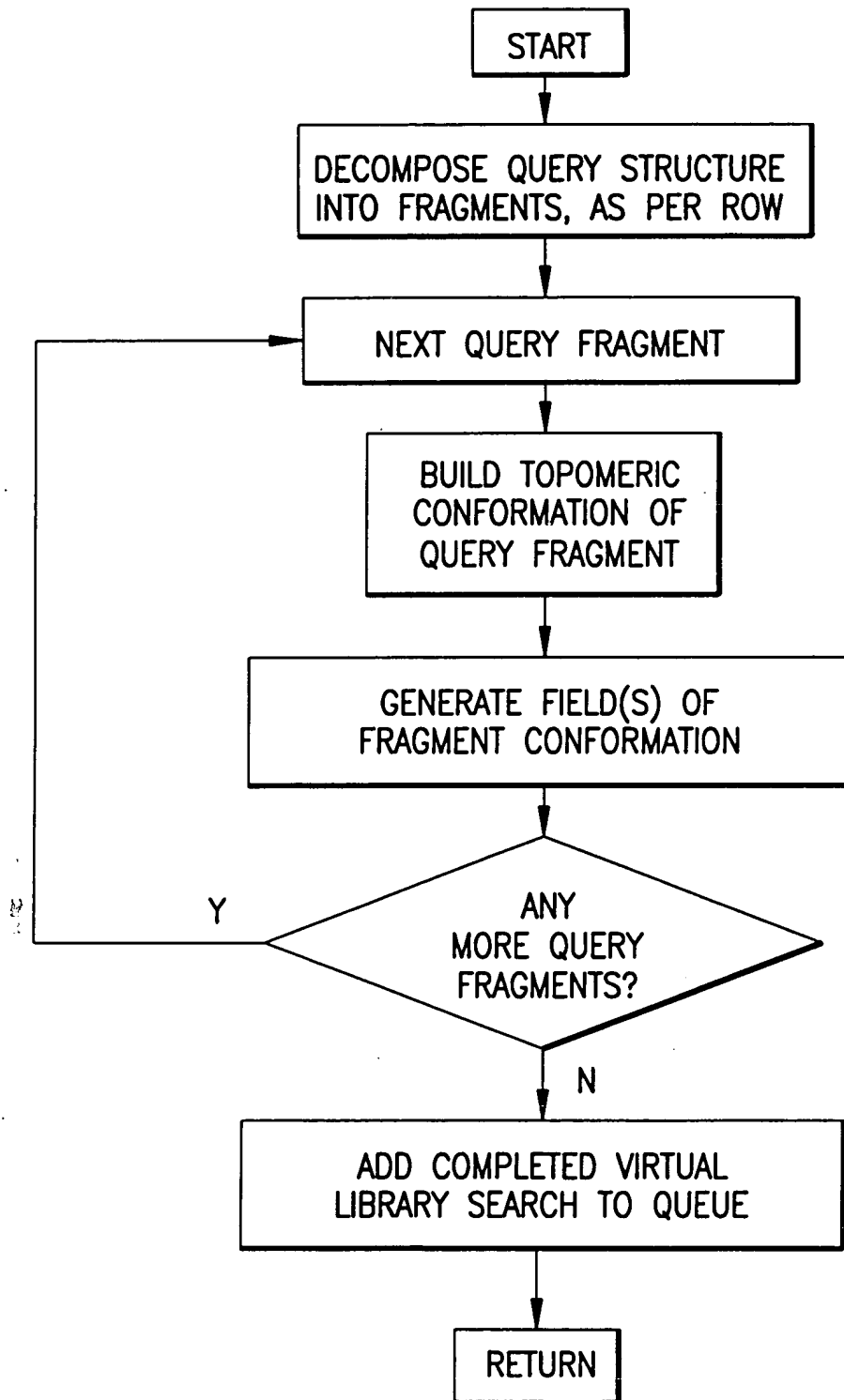


FIG.28

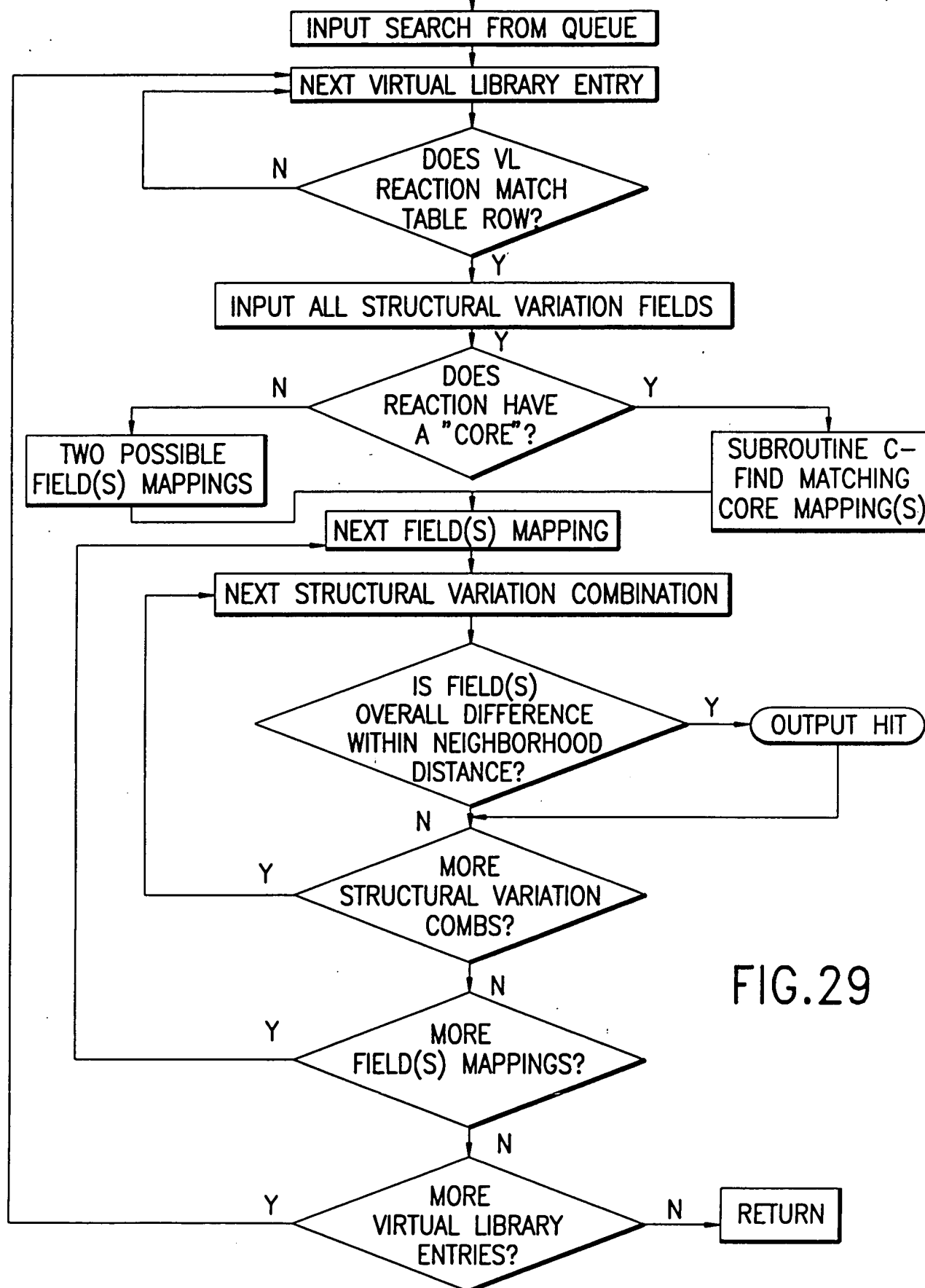


FIG.29

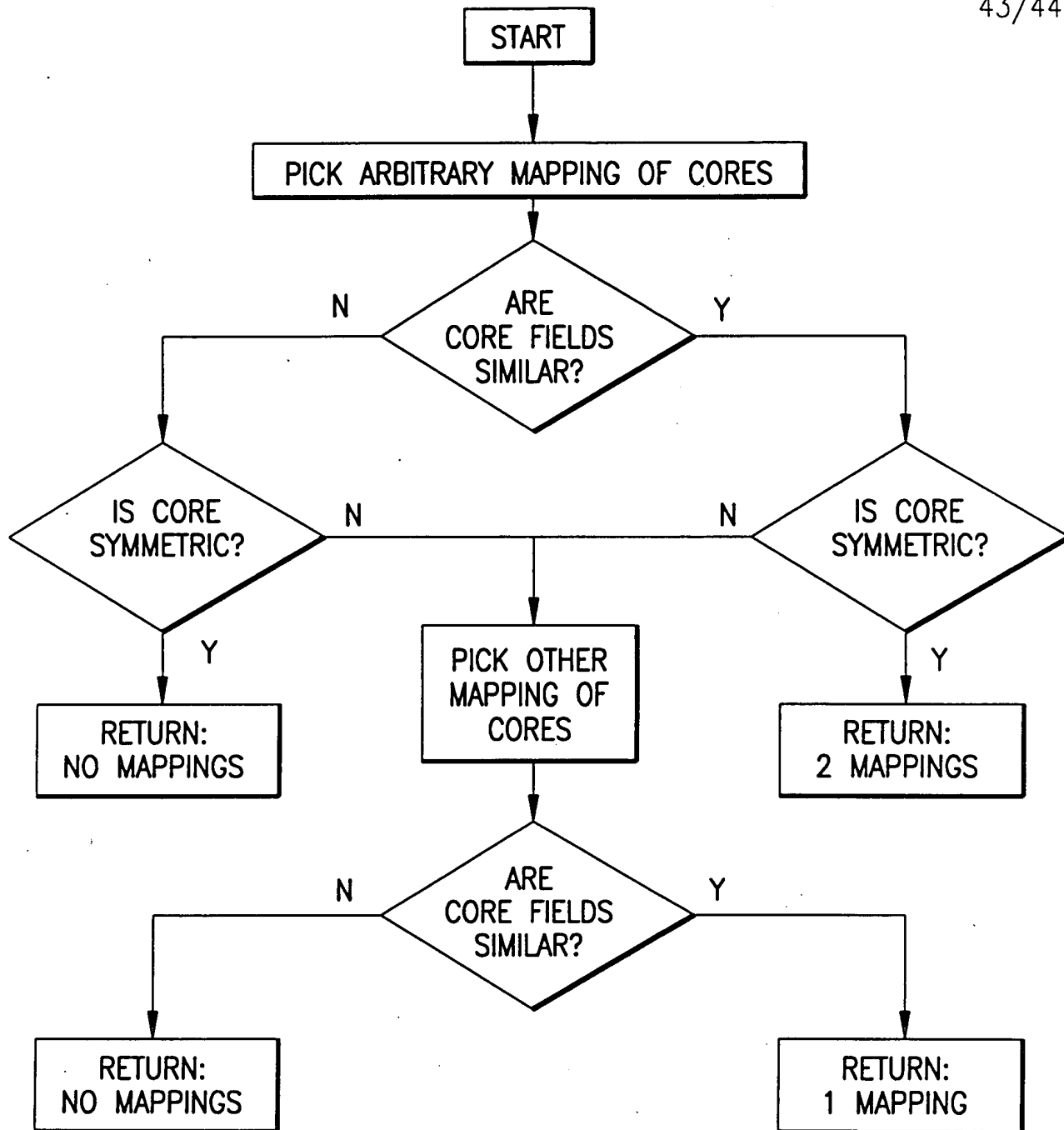


FIG.30

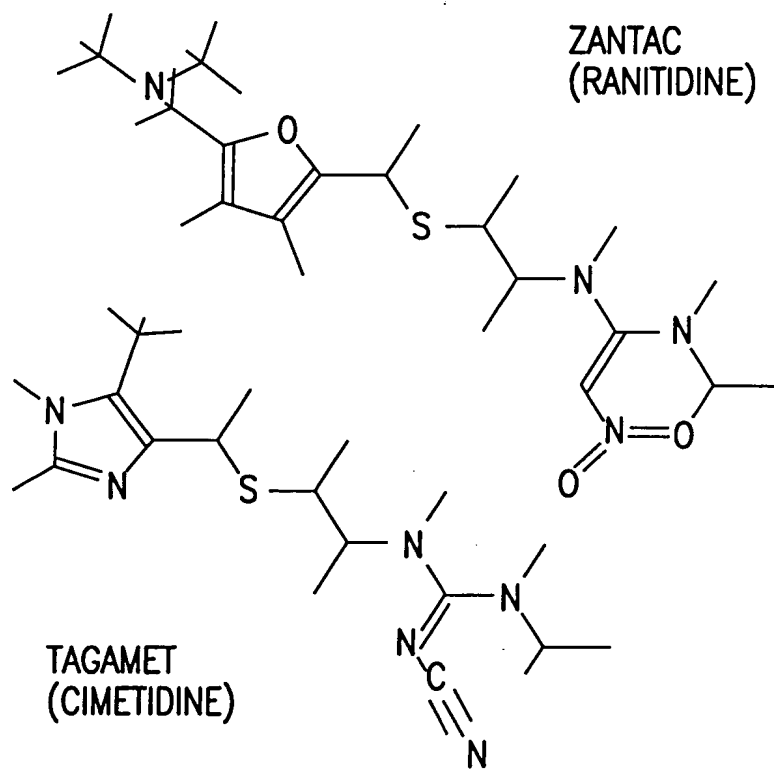


FIG.31

096544 05201
"05250" E4599860